ReaxFF: a fast, transferable computational method for atomistic-scale dynamical simulations of chemical reactions

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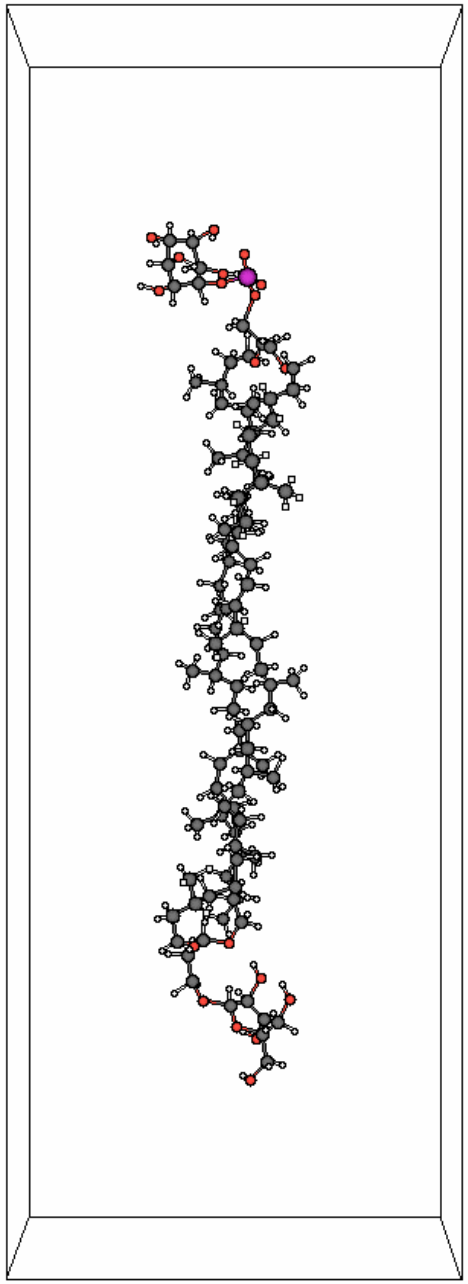
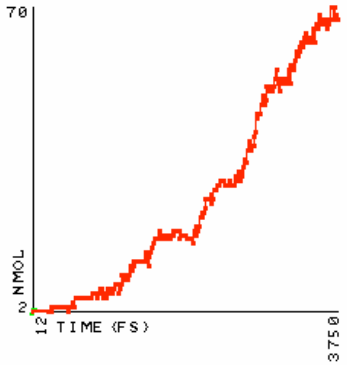
Bill Goddard

Nagarajan Vaidehi (currently City of Hope) Protein simulations	Jonas Oxgaard Catalysis	Mamadou Diallo Environmental chemistry	Sergey Zybin High-energy materials	Adri van Duin Force field development (ReaxFF)	Boris Merinov Fuel cells	Weiqiao Deng (currently U. Singapore) Nano	Andres Botero Software integration

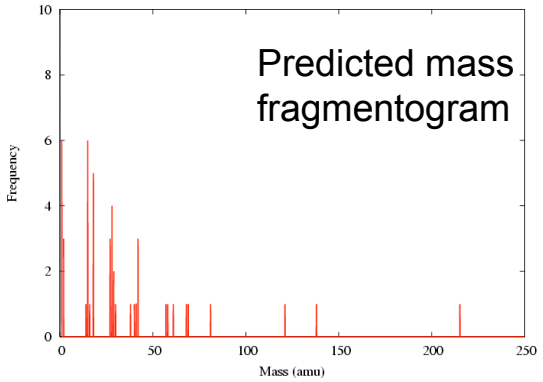
- ± 55 scientists, covering various areas of atomistic- and mesoscale simulations (QM, FF, MC)
- 60/40 government/industry funding
- Current industry projects:
  - GPCR membrane enzymes (Berlex, Avantis)
  - Methane activation (Chevron)
  - Nanotube/metal links (Intel)
  - DLC engine friction (Nissan)
  - Cu/Si catalysis (Dow Corning)
  - Semiconductors (Samsung)
- Current government-funded projects:
  - SOFC Fuel cells (DoE)
  - Stress-corrosion cracking (NSF)
  - Metaloxide catalysis (DoE)
  - Ionic liquid catalysis (DoE)
  - Explosives sensitivity (DoE, ONR)
  - Dendrimer/environment (NSF)
  - Software integration (DARPA)
  - QM-development (ASC)

What can ReaxFF do for you ?





Decomposition of a archea phospholipid biomarker (GDGT) by exposure to high-velocity (30eV) N-radicals



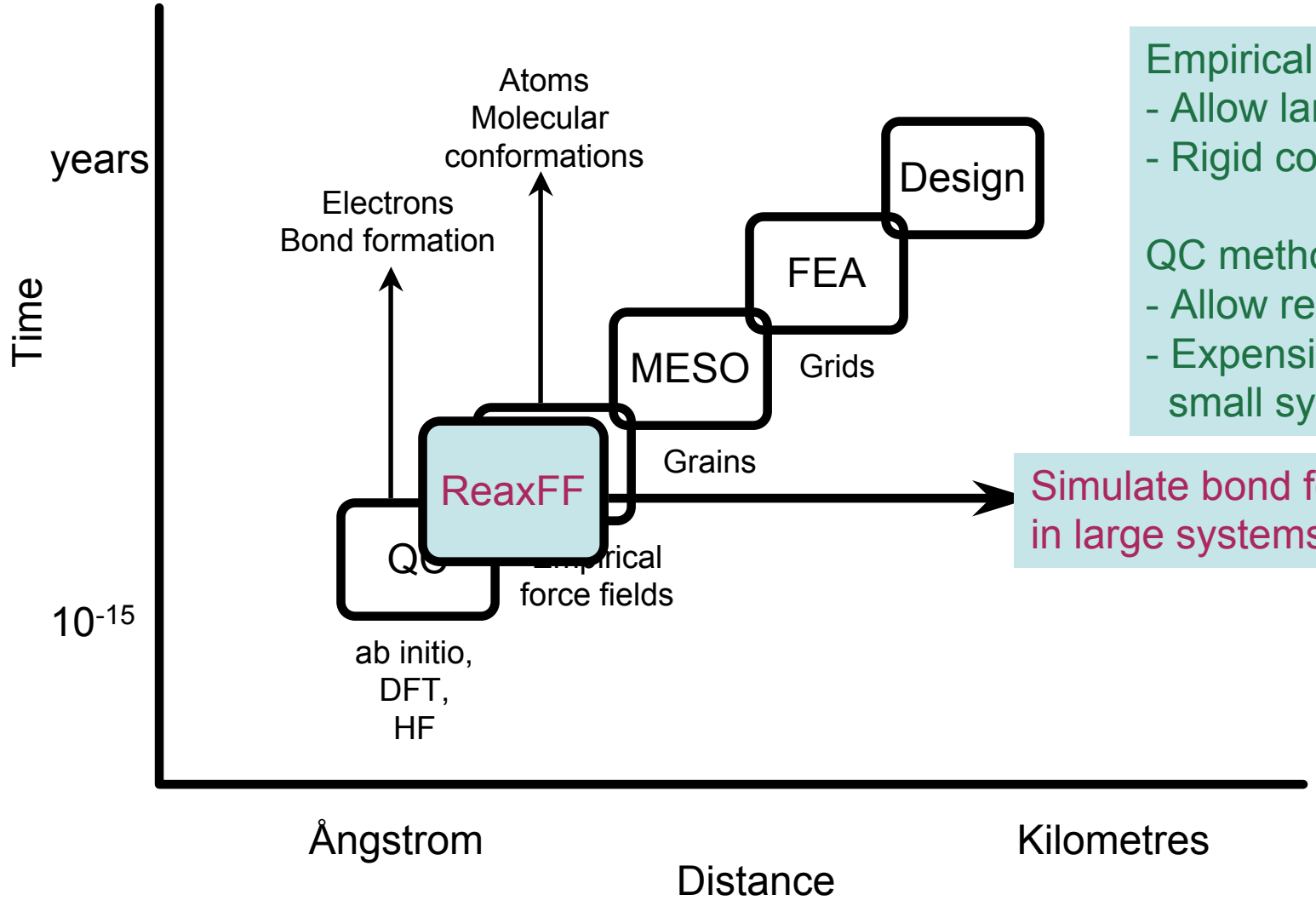
- Single-processor MD/NVE simulation
- 300-326 atoms
- 15000 MD-iterations
- CPU-time: 1884 seconds

- ReaxFF can perform fast molecular dynamics simulations involving complicated chemical reactions

Contents

- ReaxFF: background, rules and current development status
- Stress-induced crack propagation
    - Integration of ReaxFF in a multi-paradigm computational framework (CMDF)
    - ReaxFF/Tersoff/CMDF simulations on crack propagation in silicon
    - Influence of corrosion on crack propagation
- Hydrocarbon combustion and metal-oxide catalyzed hydrocarbon oxidation
    - Force field development
    - Simulations on o-Xylene combustion
    - V_2O_5-catalyzed hydrocarbon conversion
- Hydrogen and hydrocarbon conversion on Pt- and Ni-surfaces
    - Force field development
    - Methanol conversion on Pt[111]
    - Ni/Cu/Co catalyzed nanotube formation
    - H_2 dissociation on a facetted Ni_{309}-particle

ReaxFF: background and rules



Empirical methods:
- Allow large systems
- Rigid connectivity

QC methods:
- Allow reactions
- Expensive, only small systems

Simulate bond formation in large systems

ReaxFF: key features

-To get a smooth transition from nonbonded to single, double and triple bonded systems ReaxFF employs a bond length/bond order relationship[1,2]. Bond orders are updated every iteration.

- Nonbonded interactions (van der Waals, Coulomb) are calculated between every atom pair, irrespective of connectivity. Excessive close-range nonbonded interactions are avoided by shielding.

- All connectivity-dependent interactions (i.e. valence and torsion angles) are made bond-order dependent, ensuring that their energy contributions disappear upon bond dissociation.

- ReaxFF uses a geometry-dependent charge calculation scheme that accounts for polarization effects.

[1]:Tersoff, PRB 1988;[2]: Brenner PRB 1990

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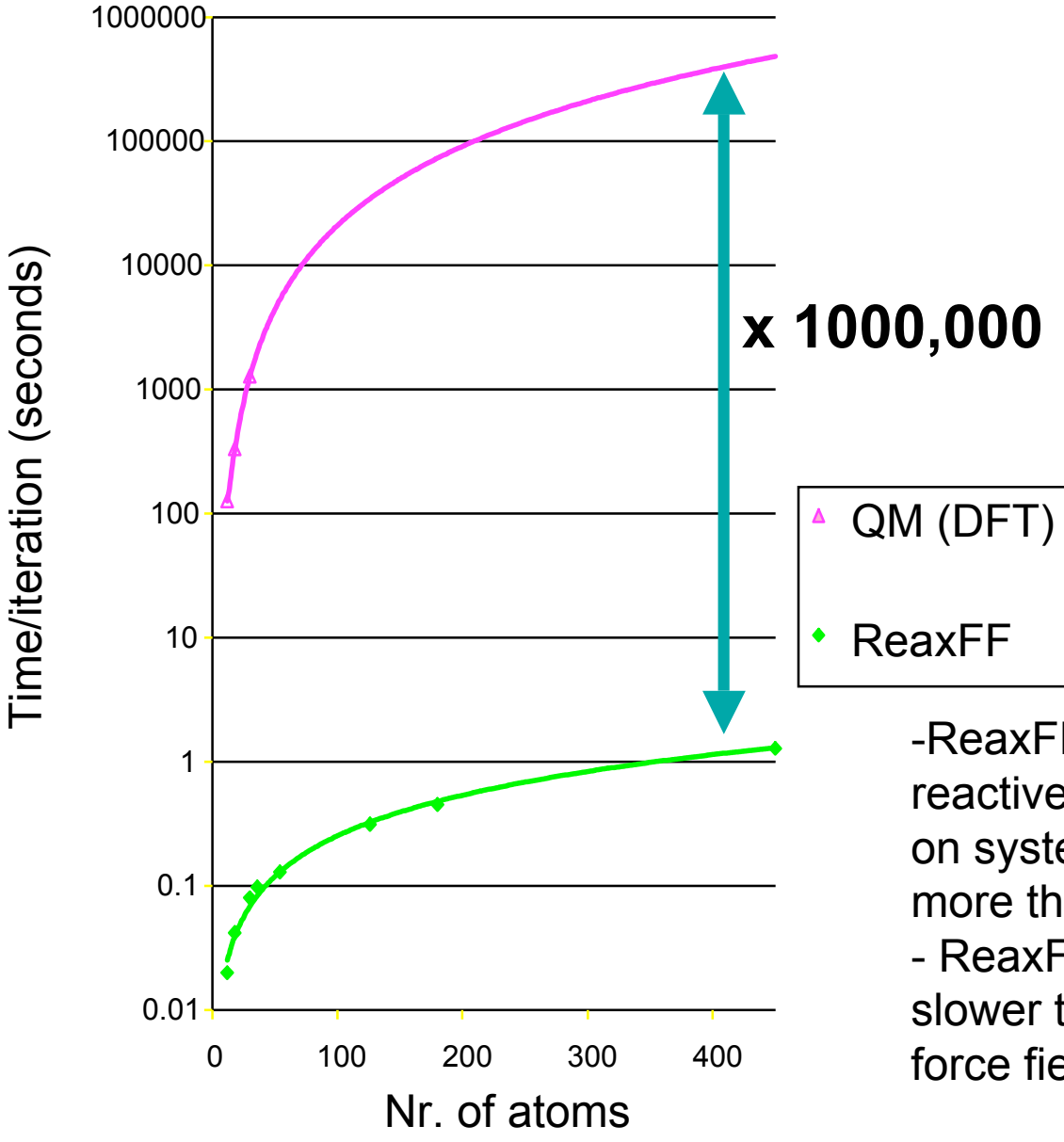
General rules

- MD-force field; no discontinuities in energy or forces even during reactions.

- User should not have to pre-define reactive sites or reaction pathways; potential functions should be able to automatically handle coordination changes associated with reactions.

- Each element is represented by only 1 atom type in the force field; force field should be able to determine equilibrium bond lengths, valence angles etc. from chemical environment.

ReaxFF Computational expense



-ReaxFF allows for reactive MD-simulations on systems containing more than 1000 atoms
- ReaxFF is 10-50 times slower than non-reactive force fields

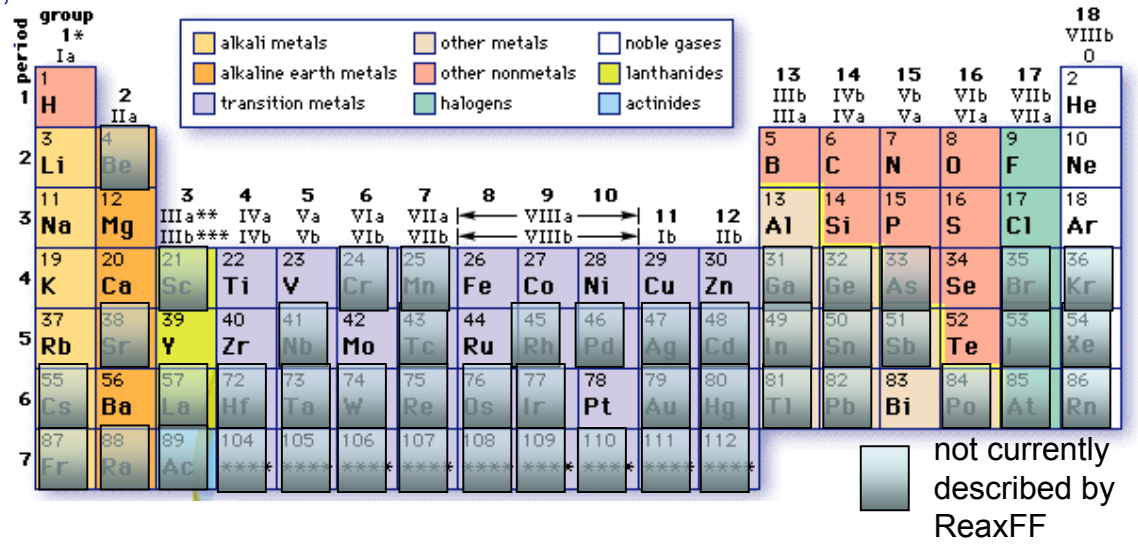
Current development status

Published ReaxFF force fields for:

- H/C (van Duin, Dasgupta, Lorant and Goddard, JPC-A 2001, **105**, 9396; van Duin and Sinninghe Damste, Org. Geochem.2003, **34**, 515; Chen, Lusk, van Duin and Goddard PR-B 2005, **72**, 085416, Han, Kang, Lee, van Duin and Goddard Appl. Phys. Lett. 2005, **86**, 203108)
- $Si/SiO_2/SiC$ (van Duin, Strachan, Stewman, Zhang, Xu and Goddard, JPC-A 2003, **107**, 3803; Chenoweth, Cheung, van Duin, Goddard and Kober, JACS 2005, **127**, 7192; Buehler, van Duin and Goddard, PRL 2006, **96**, 095505)
- Nitramines/RDX/TATP (Strachan, van Duin, Chakraborty, Dasupta and Goddard, PRL 2003,**91**,09301; Strachan, van Duin, Kober and Goddard, JCP 2005,**122**,054502; Han, Strachan, van Duin and Goddard, in preparation; van Duin, Dubnikova, Zeiri, Kosloff and Goddard, JACS 2005, **127**, 11053)
- Al/Al_2O_3 (Zhang, Cagin, van Duin, Goddard, Qi and Hector, PRB 2004,**69**,045423)
- Ni/Cu/Co/C (Nielson, van Duin, Oxgaard, Deng and Goddard, JPC-A 2005, **109**, 493)
- Pt/PtH (Ludwig, Vlachos, van Duin and Goddard, JPC-B 2006)
- Mg/MgH (Cheung, Deng, van Duin and Goddard, JPC-A 2005, **109**, 851)
- BN-nanotubes (Han, Kang, Lee, van Duin and Goddard, JCP 2005, **123**,114703; Han, Kang, Lee, van Duin and Goddard, JCP 2005, **123**,114704)
- Li/LiC (Han, van Duin and Goddard, JPC-A 2005, **109**. 4575)

Force fields in development for:

- Other transition metals, metal alloys
- Proteins, organic phosphates
- Ionic liquids (imidazole/BF_4/PF_6)
- Code has been distributed to over 30 research groups
- Parallel ReaxFF (GRASP/Reax and USC/Reax)



Parallel ReaxFF: GRASP/ReaxFF

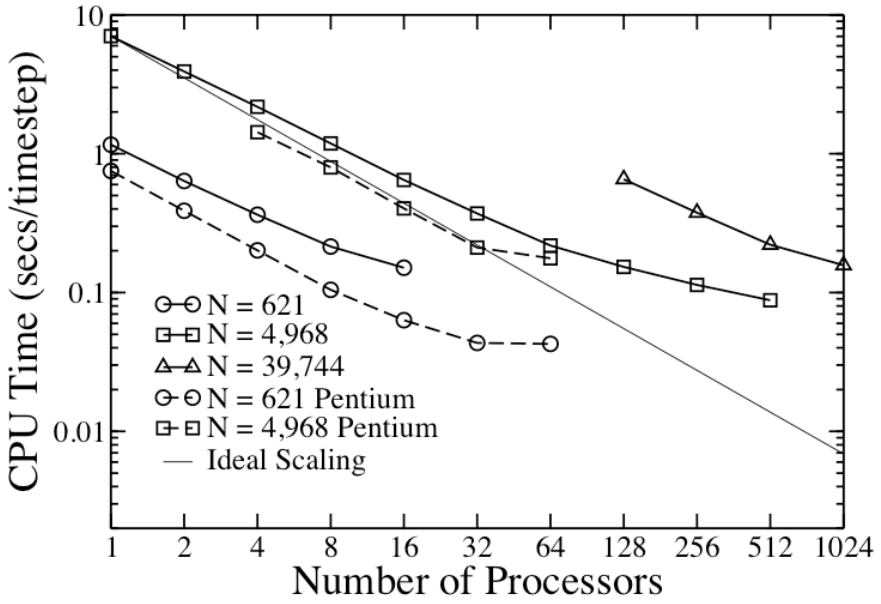
- ReaxFF is now incorporated in the Grasp-framework (Aidan Thompson, Sandia) allowing parallel ReaxFF-simulations.

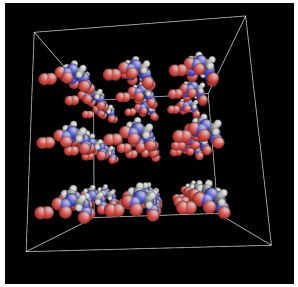
GRASP Performance on BG/L with ReaxFF

Comparison with Liberty Cluster (3GHz Pentium+Myrinet)

RDX Explosive with Oxygen

ReaxFF force field with charge equilibration





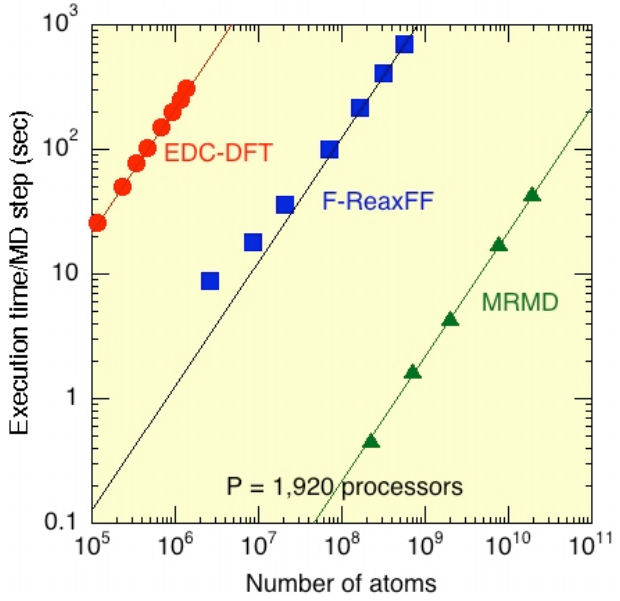
- ReaxFF enables reactive modelling
- Si/SiO_2, Explosives, film growth
- Each process computes energy and forces for a virtual non-periodic cluster
- Low communication, duplicated computation ~ $P(N/P)^{2/3}$
- Uses Van Duin's Fortran subroutines for force calculation.
- Good strong scaling
- Sweet spot: 5000 atoms/processor

Parallel ReaxFF: USC-Caltech-Ames collaboration

USC-Caltech-NASA Ames collaboration

Design-space diagram on 1,920 Itanium2 (1.5GHz) procs. of NASA Columbia

Collaborators: R. Biswas, D. Srivastava (NASA-Ames)



Parallel efficiency as high as 0.953

- 19 billion-atom classical multiresolution MD (MRMD) of SiO_2
- 0.56 billion-atom fast reactive force-field (F-ReaxFF) MD of RDX
- 1.4 million-atom (0.12 trillion grid points) embedded divide-&-conquer (EDC)-density functional theory (DFT) MD of Al_2O_3

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A divide-and-conquer/cellular-decomposition framework for million-to-billion atom simulations of chemical reactions

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[b] Department of Physics, Kumamoto University, Kumamoto 860-8555, Japan
[c] Materials and Process Simulation Center, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA 91125, USA
[d] NASA Advanced Supercomputing (NAS) Division, NASA Ames Research Center, Moffett Field, CA 94035, USA

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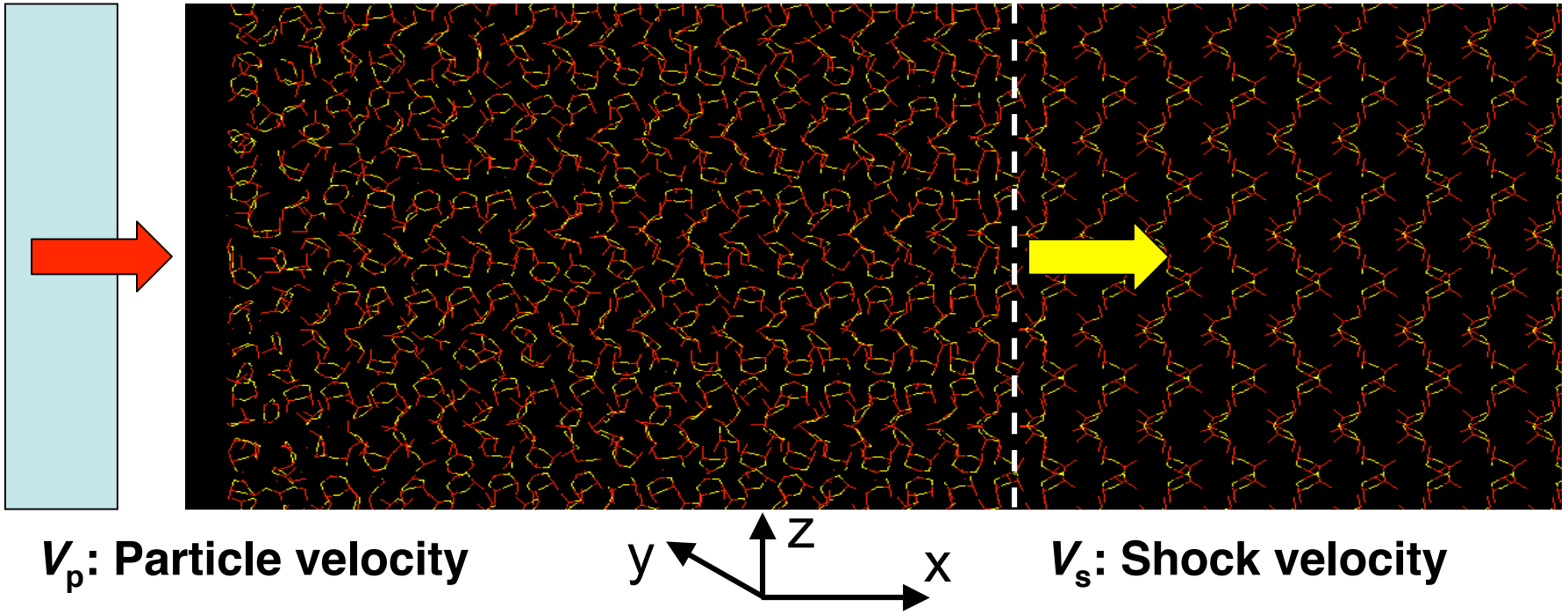
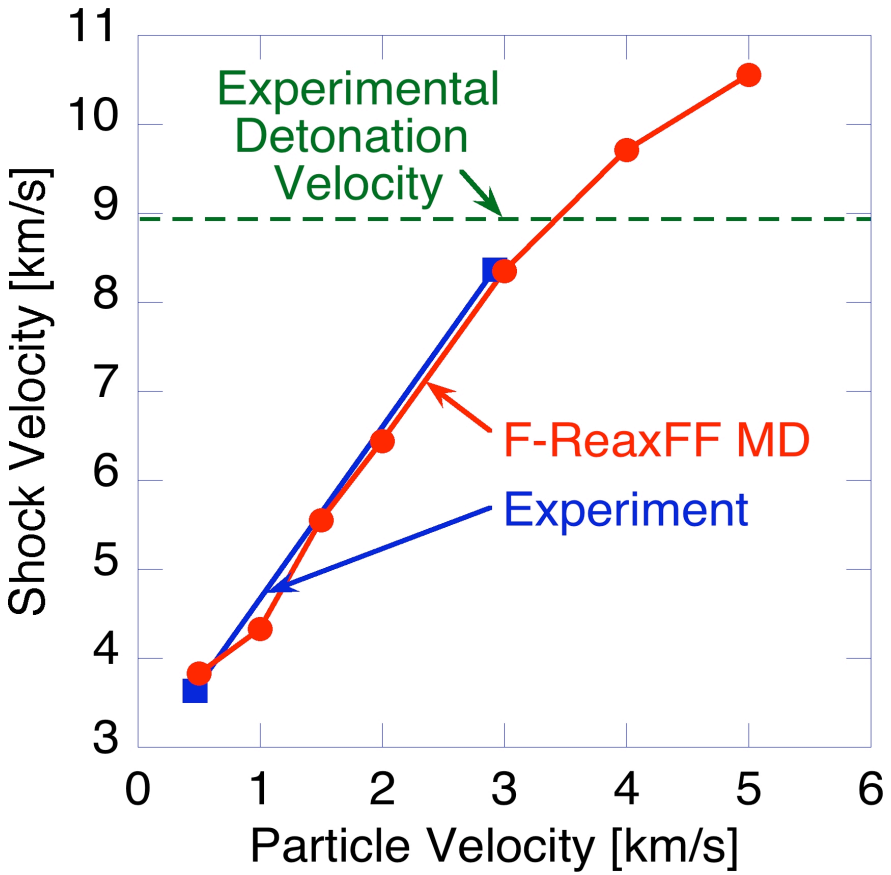
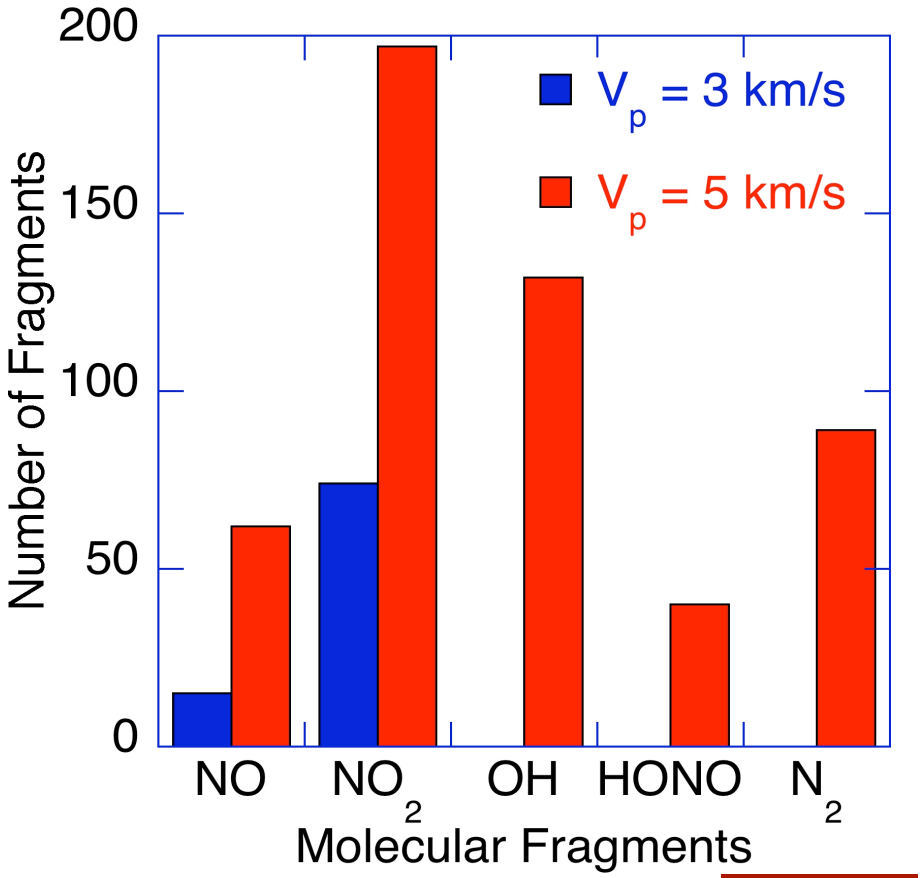
Planar Shock on RDX Crystal



- USC's parallel F-ReaxFF program
- Number of atoms: 2,322,432 or 145,152
- System size: 358×284×271 Å^3 (24×24×24 unit cells) or
  358×71×68 Å^3 (24×6×6 unit cells)
- Particle velocity: $V_p = 0.5–5$ (km/s)
- Piston modeled as a momentum mirror

Planar Shock on RDX





- Shock velocity agrees well with experimental data
- Onset of detonation consistent with the experimental detonation velocity

- ReaxFF: background, rules and current development status
- Stress-induced crack propagation
    - Developing the Si/SiO reactive force field
    - Stress-induced crack propagation
    - Integration of ReaxFF in a multi-paradigm computational framework (CMDF)
    - ReaxFF/Tersoff/CMDF simulations on crack propagation in silicon
    - Influence of corrosion on crack propagation
- Hydrocarbon combustion and metal-oxide catalyzed hydrocarbon oxidation
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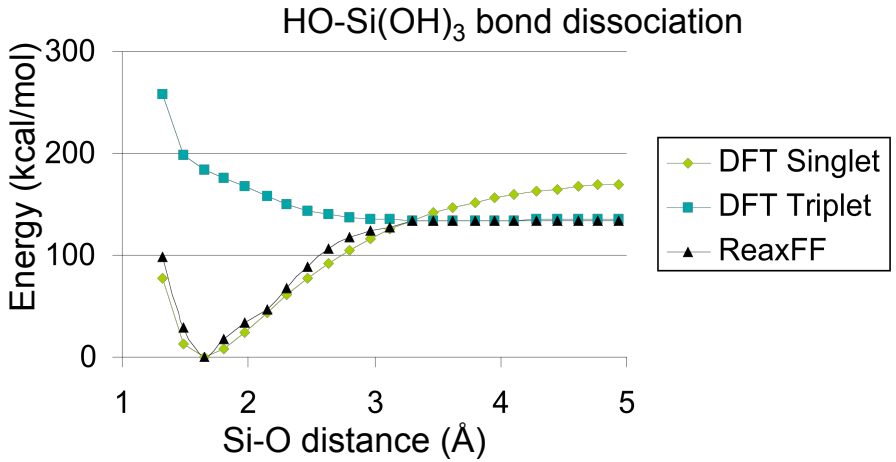
Developing the Si/SiO reactive force field

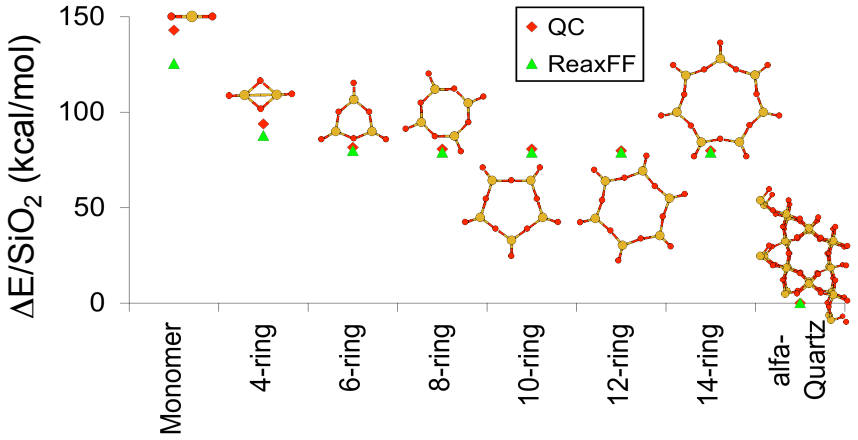
1) Bond dissociation energies



Other cases :Si-Si, Si=Si, Si=O, Si-H, O-O, O=O, O-H

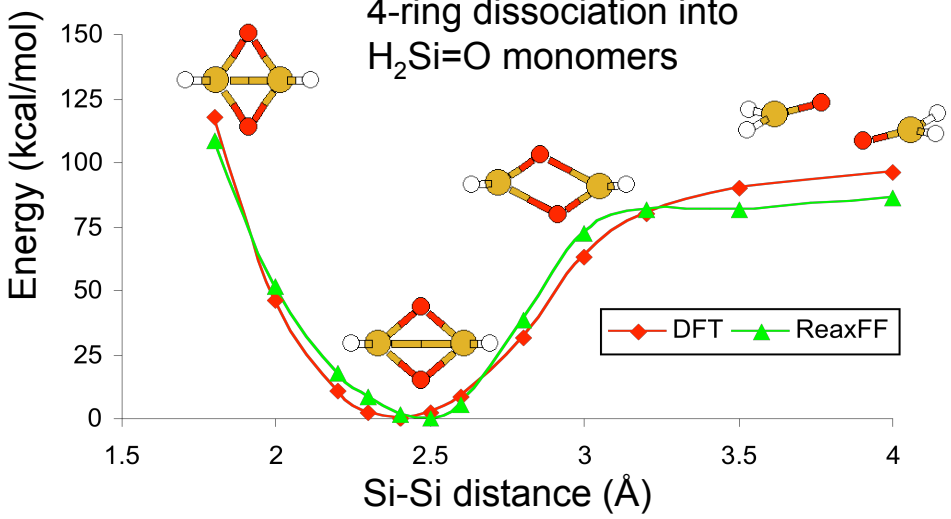
2) Angle strain

Ring size/strain correlation in SiO_2-polymers



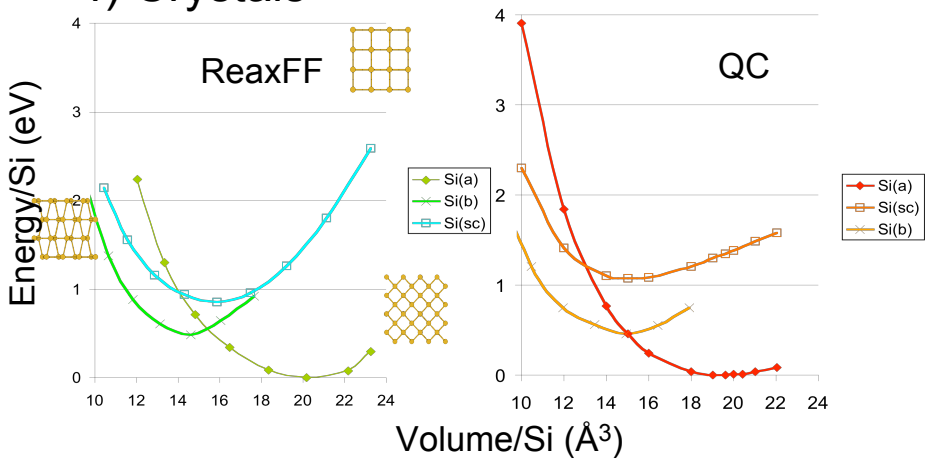
Other cases: Si/O/H angle bending energies, SiO and SiH_2-six membered ring deformation energy

3) Reactions



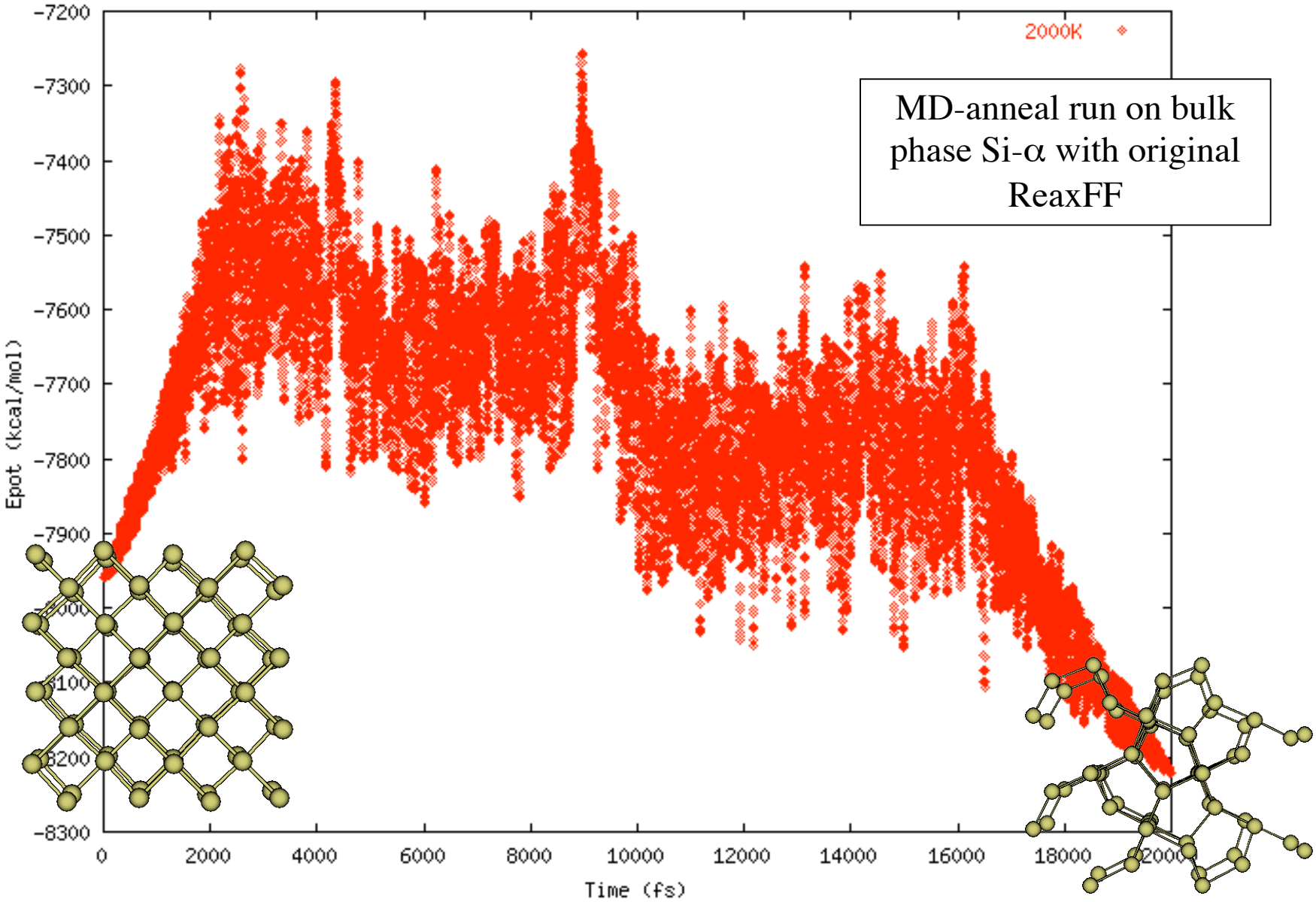
Other cases: Condensation reactions, H_2O incorporation into Si-surfaces

4) Crystals



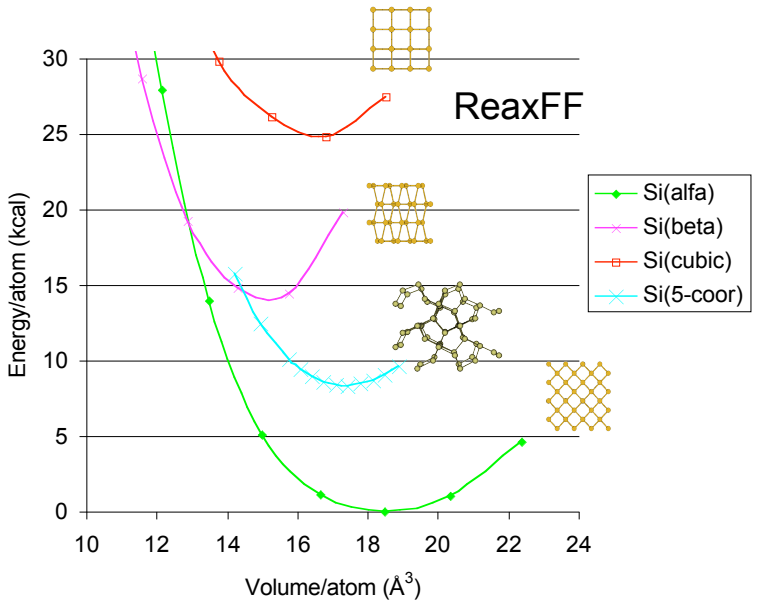
Other cases: Equations of state and relative stability of SiO_2-polymorphs, including high-pressure phases like stishovite, $CaCl_2$ and PbO_2

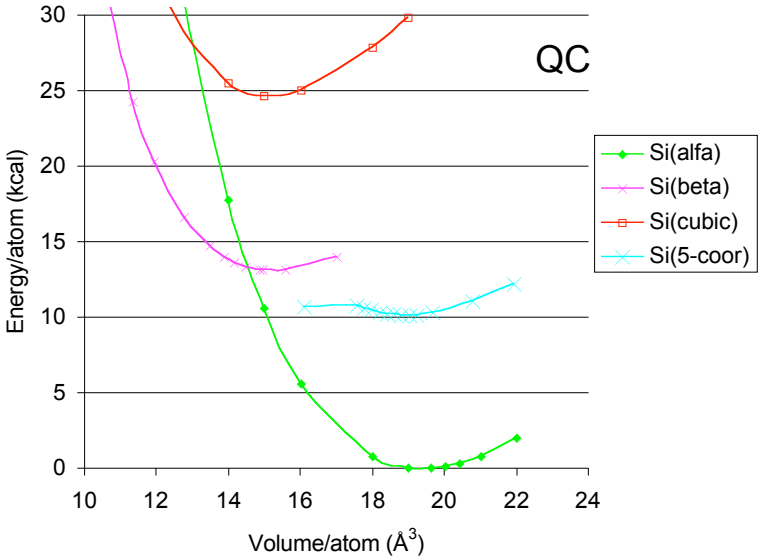
Correcting a ‘finished’ ReaxFF force field



- Original ReaxFF overstabilizes 5-coordination for silicon bulk phase

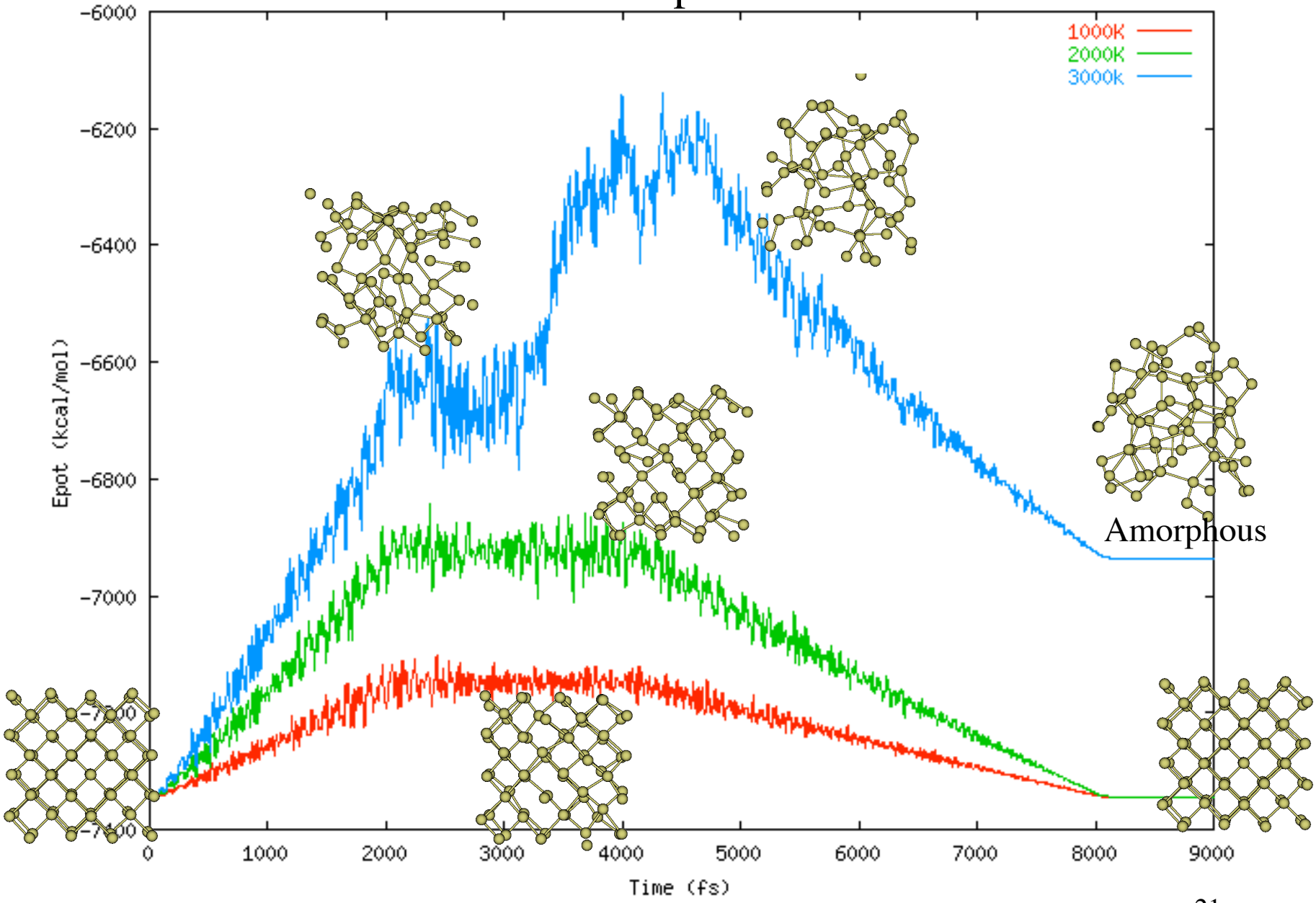
Re-optimize ReaxFF with equation of state for 5-coordinate Si-phase





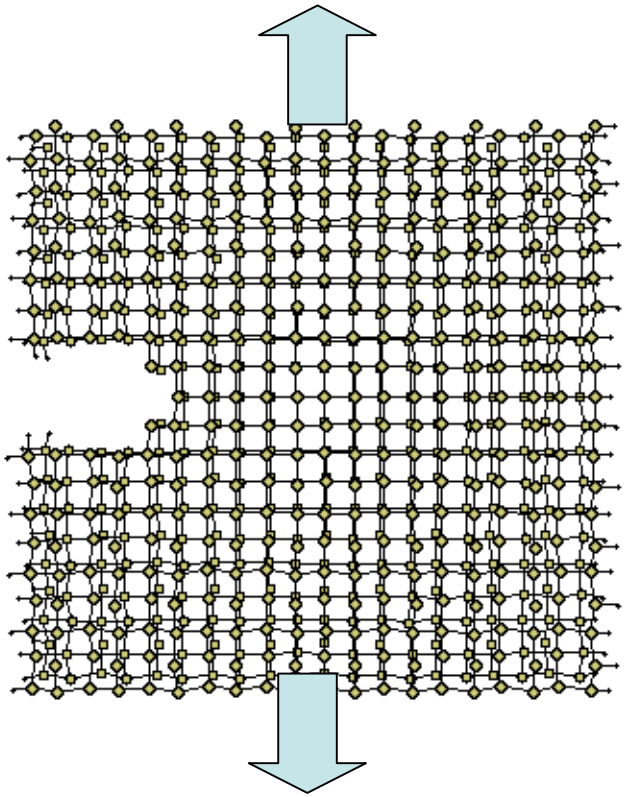
- Re-optimized ReaxFF gets proper stability for 5-coordinate Si-phase
- 5-coordinate phase is more stable than 6-coordinate Si(β) !
- 5-coordinate Si might be important in amorphous Si

MD-anneal run on bulk phase Si-α with ReaxFF



Stress-induced crack propagation

with Markus Buehler (MIT), Jef Dodson, Si-ping Han, Yi Liu, Andres Jaramillo Botero and Bill Goddard

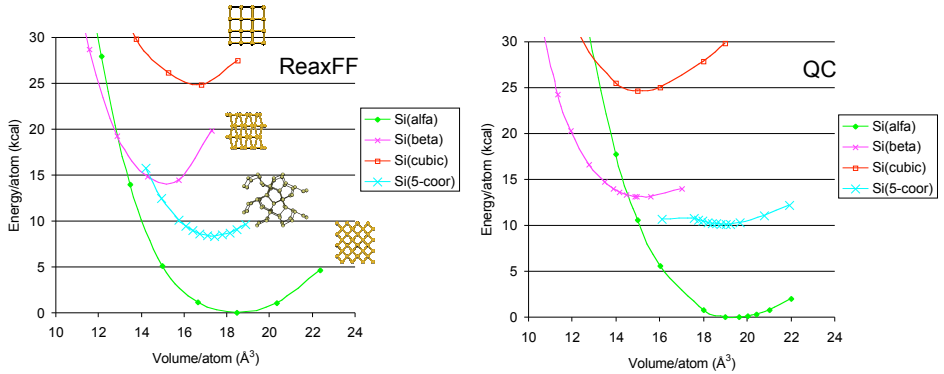


Hydrogen-terminated Si-slab
ReaxFF NVT (100K) MD-simulation

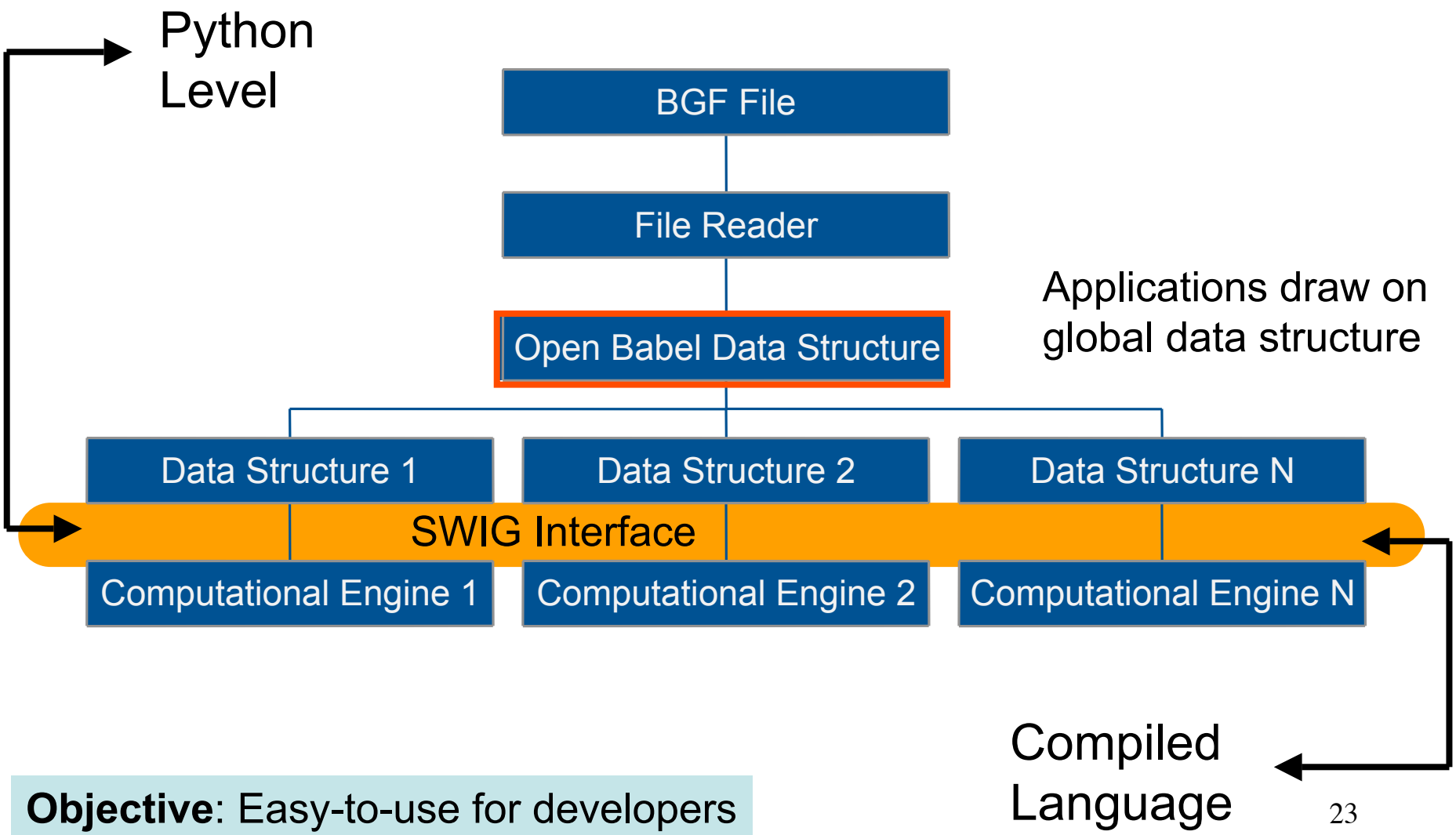
- ReaxFF describes proper, brittle behaviour of crack propagation in silicon
- ReaxFF can be used to simulate effects of corrosive reactants (H_2O, H_3O^+, O_2) on crack propagation speed
- ReaxFF is 20-50 times slower than non-reactive metal or metal oxide FF

- Use ReaxFF at crack-tip and metal/metal oxide interface; use cheaper method away from reactive zone

ReaxFF and QM equations of state for Si

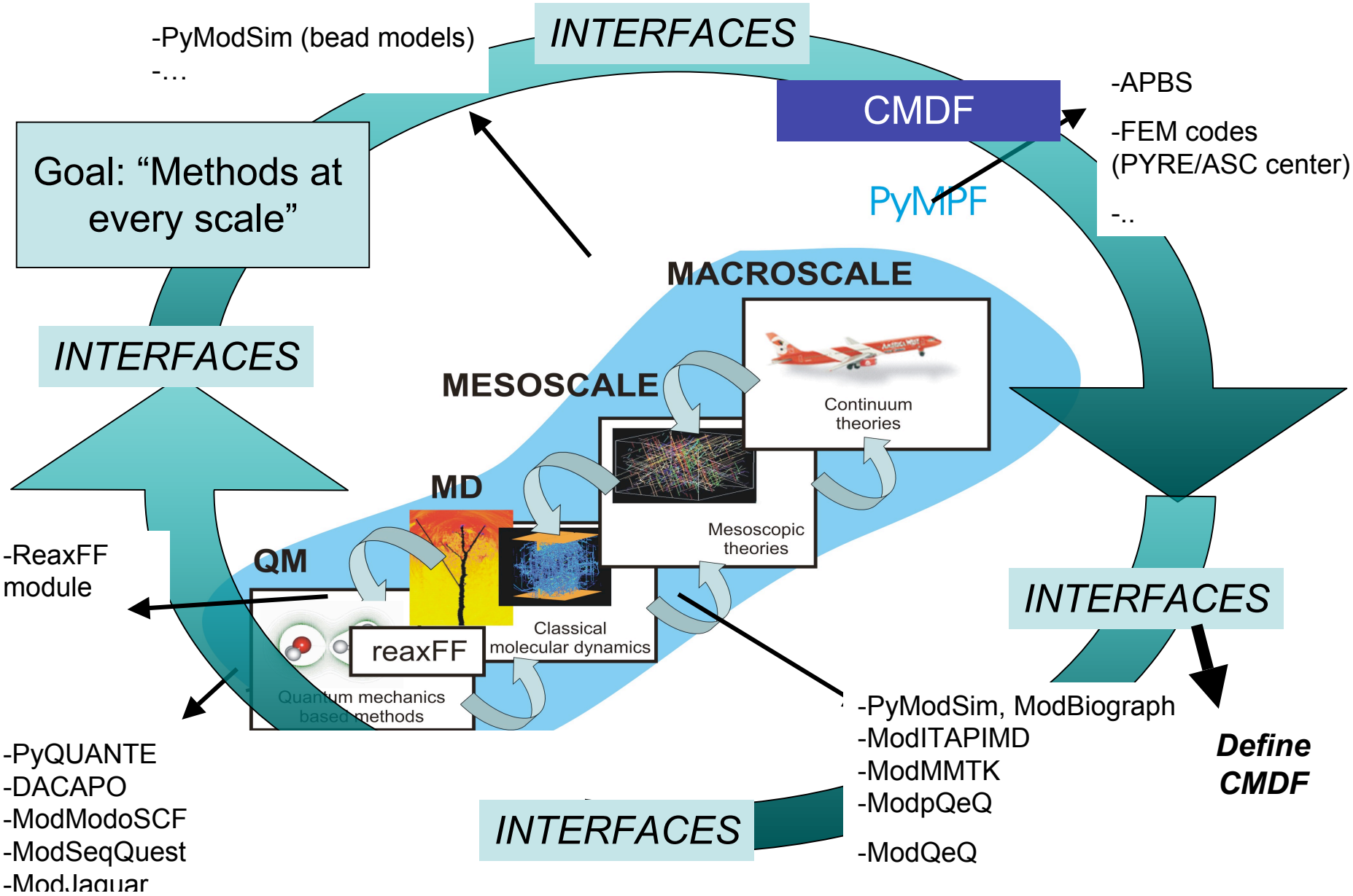


Integration of ReaxFF in a multi-paradigm computational framework (CMDF)



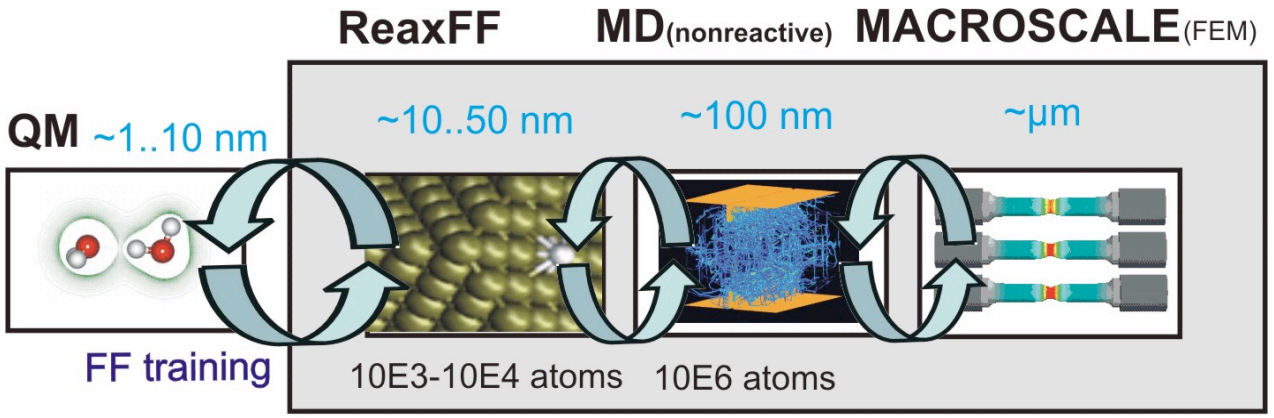
Objective: Easy-to-use for developers

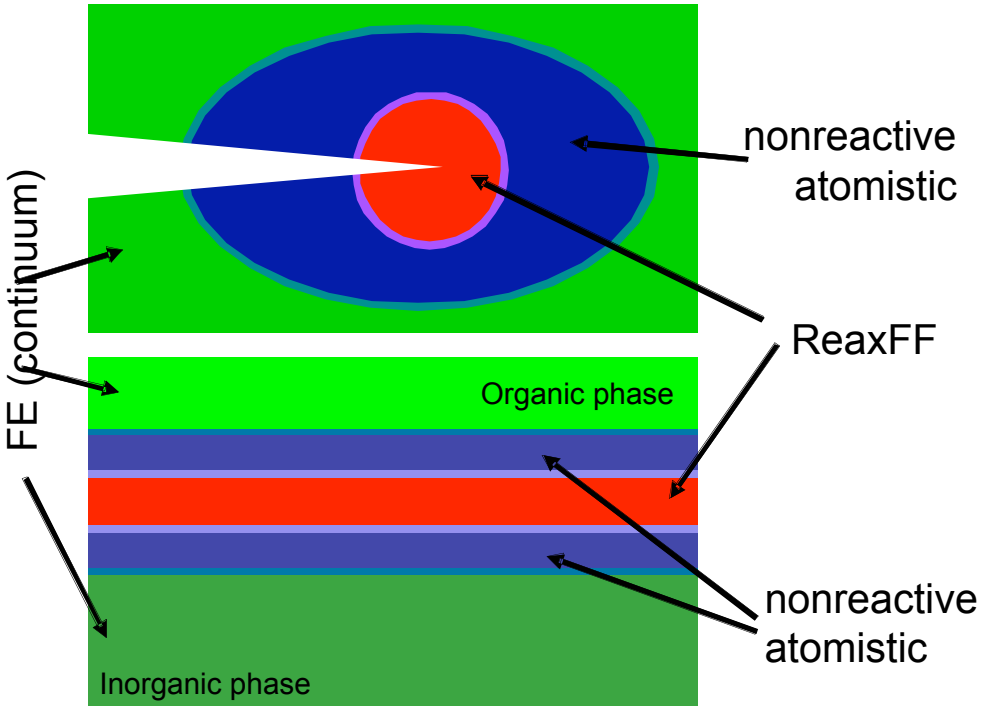
Current simulation methods in CMDF



Multi-scale simulations on crack-propagation

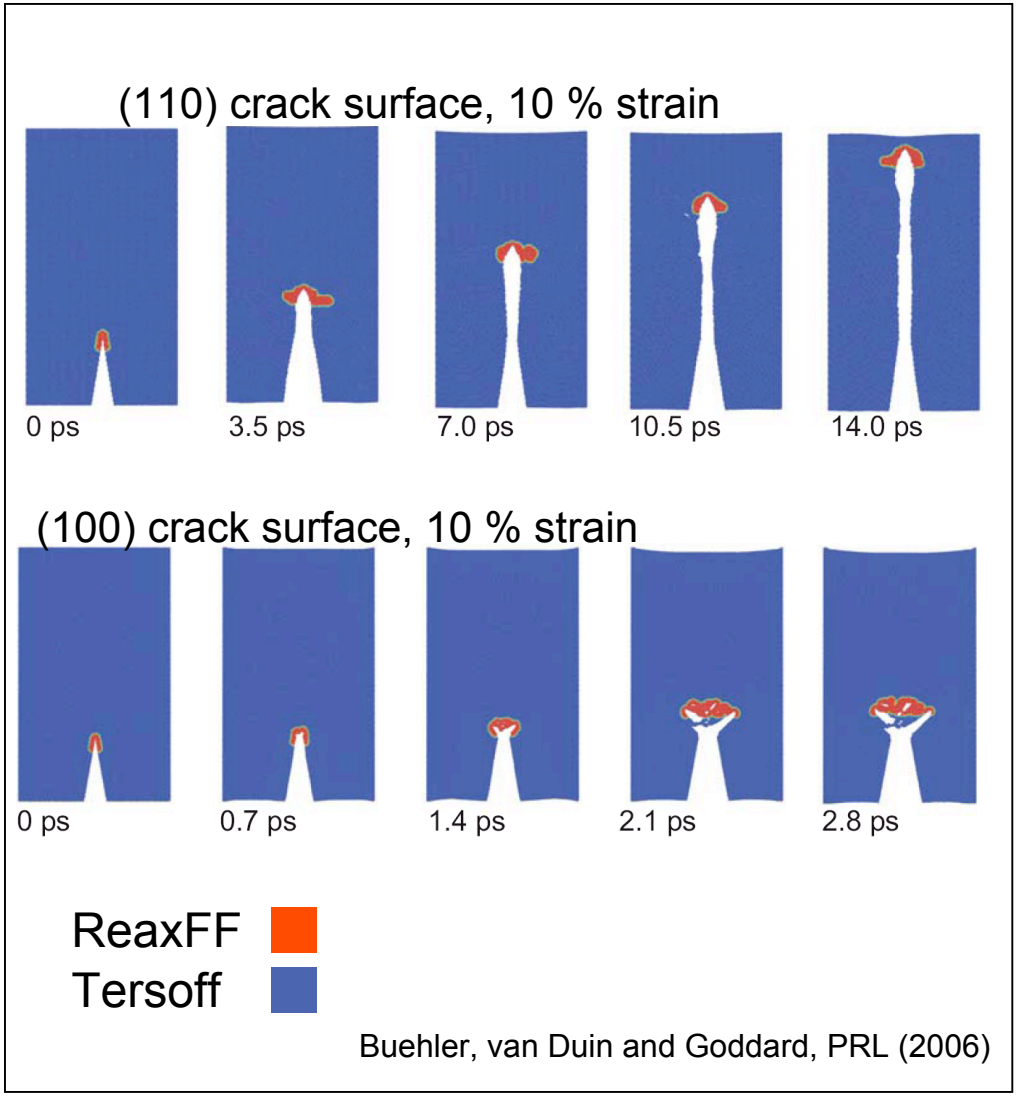
Concurrent integration of various scales and paradigms



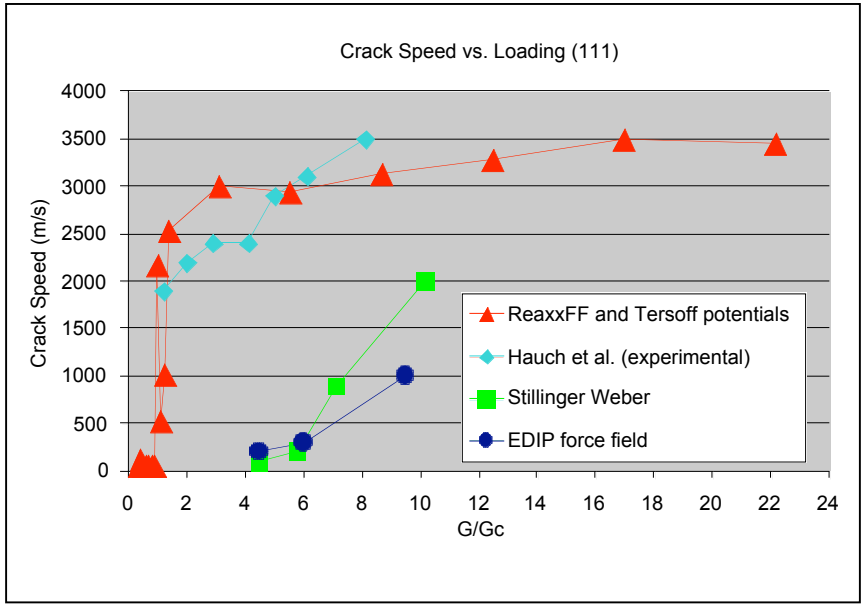


- Concurrent FE-atomistic-ReaxFF scheme in a crack problem (crack tip treated by ReaxFF) and an interface problem (interface treated by ReaxFF).
- Highlighted transition regions as handshake domains between different scale and methods.
- QM stays out of multi-scale simulation; use QM to train ReaxFF

ReaxFF/CMDF application to crack propagation in silicon



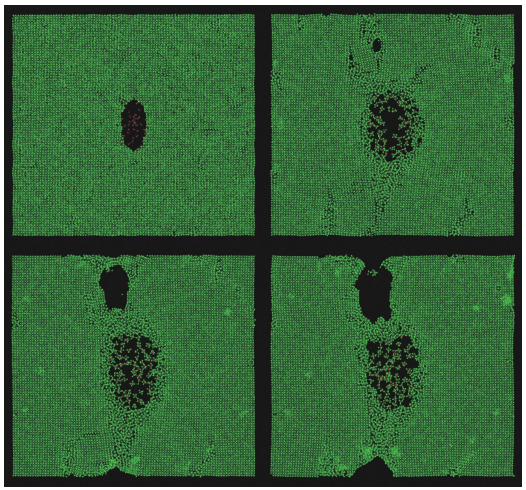
Buehler, van Duin and Goddard, PRL (2006)



- Excellent agreement with experiment
- ReaxFF can predict material properties not covered specifically by its QM-training set

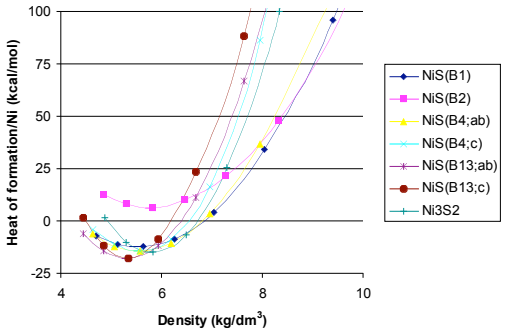
Influence of corrosion on crack propagation

ReaxFF/EAM/CMDF simulations



Influence of oxidation on crack propagation in aluminium

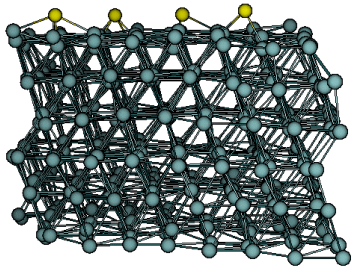
QM



Determine equations of state, binding energies, barriers

training

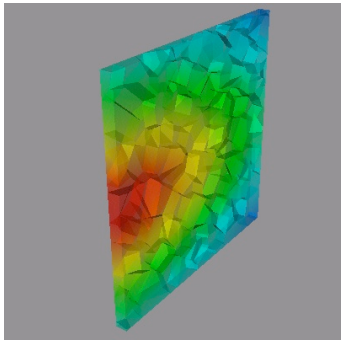
ReaxFF



Determine sulfur diffusion constants and decohesion behaviour in Ni-bulk, surfaces and grains

training

Finite element



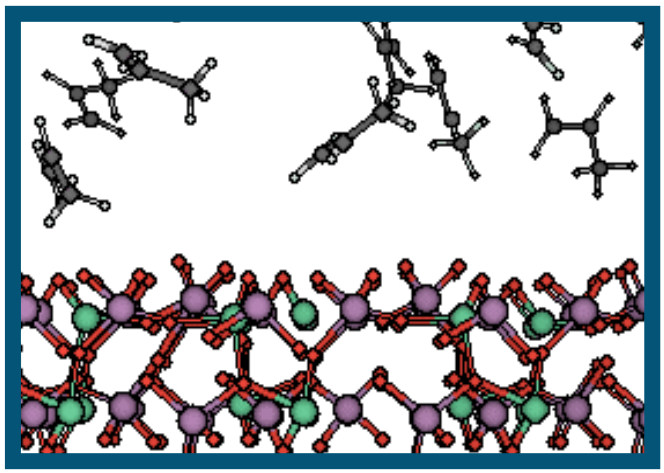
Simulation of stress-corrosion in macroscopic samples

Collaboration with Ortiz-group (Caltech) and Vashishta-group (USC)

- ReaxFF: background, rules and current development status
- Stress-induced crack propagation
    - Integration of ReaxFF in a multi-paradigm computational framework (CMDF)
    - ReaxFF/Tersoff/CMDF simulations on crack propagation in silicon
    - Influence of corrosion on crack propagation
- Hydrocarbon combustion and metal-oxide catalyzed hydrocarbon oxidation
    - Force field development
    - Simulations on o-Xylene combustion
    - V_2O_5-catalyzed hydrocarbon conversion
- Hydrogen and hydrocarbon conversion on Pt- and Ni-surfaces
    - Force field development
    - Methanol conversion on Pt[111]
    - Ni/Cu/Co catalyzed nanotube formation
    - H_2 dissociation on a facetted Ni_{309}-particle

Hydrocarbon oxidation

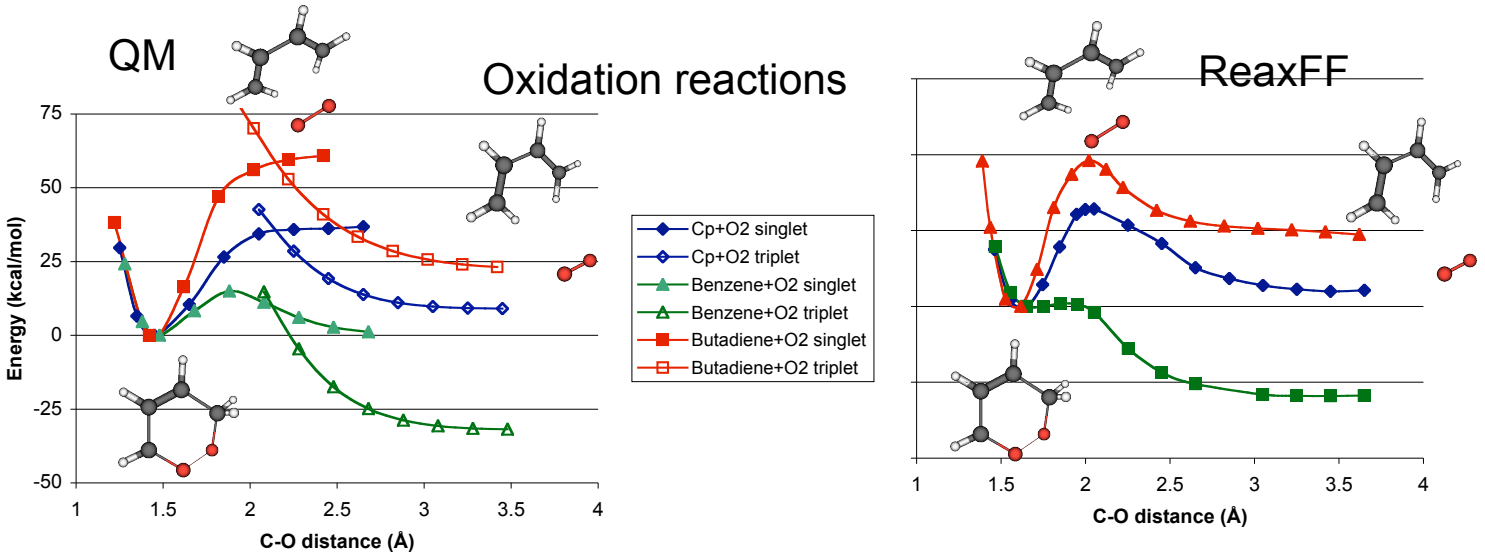
with Kimberly Chenoweth, Sanja Pudar, Mu-Jeng Cheng, Jonas Oxgaard and Bill Goddard



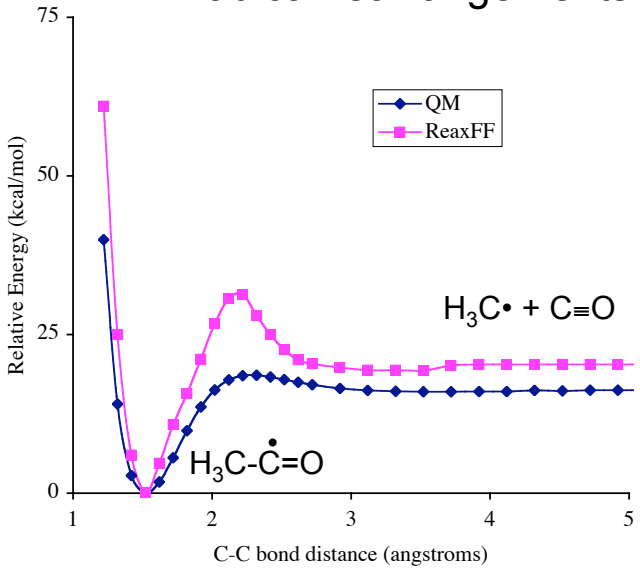
Mixed metal oxide catalyst ($Bi_xMo_yV_zTe_aO_b$)

- Selective oxidation of propene using multi-metal oxide (MMO) catalysts
  - Accounts for majority of the 8 billion pounds of acrolein produced annually (4-5% yearly growth)
- Small improvements in catalytic efficiency can have major impact on energy requirements
- Understanding the process on a molecular level required to improve efficiency and/or selectivity
- Complicated structure MMO-catalysts make QM very expensive
- Develop ReaxFF based on QM-data , use ReaxFF to perform high-temperature simulations on catalyst/hydrocarbon reactions
- First, need to establish that ReaxFF can describe non-catalytic hydrocarbon combustion

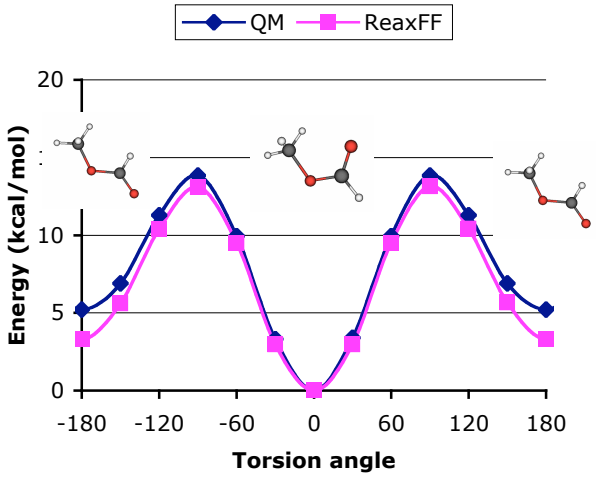
Force field development: hydrocarbon oxidation



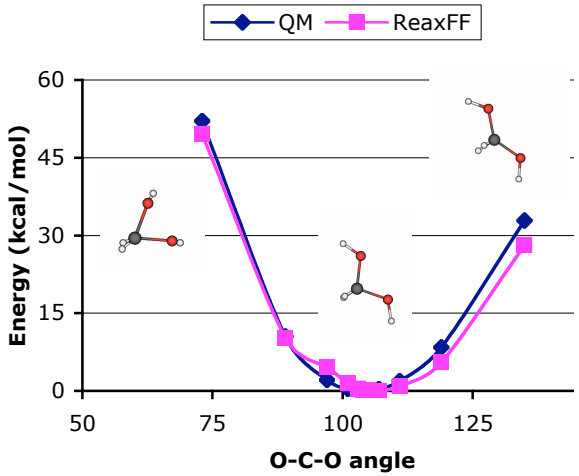
Radical rearrangements



Rotational barriers

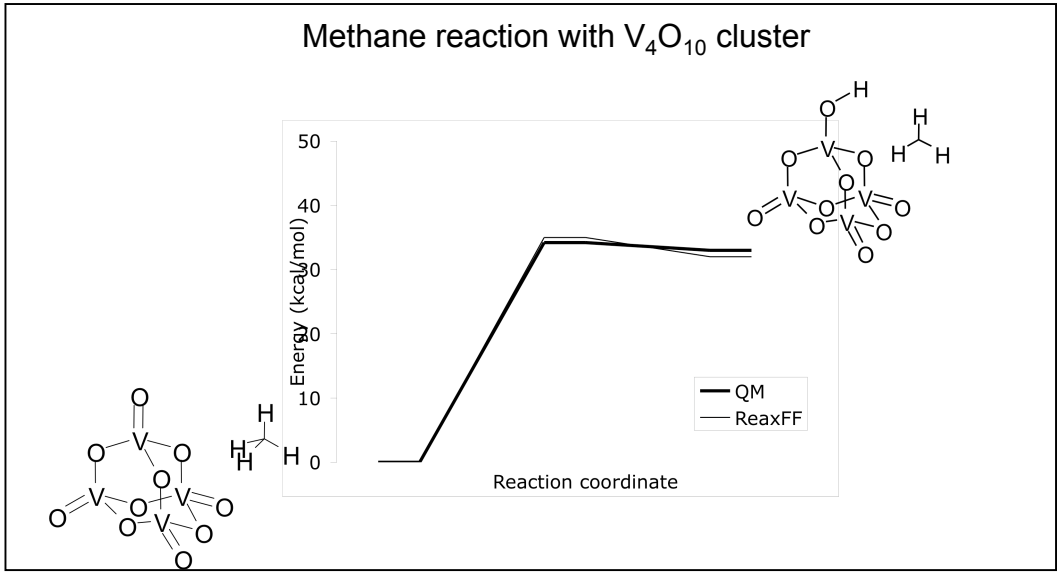


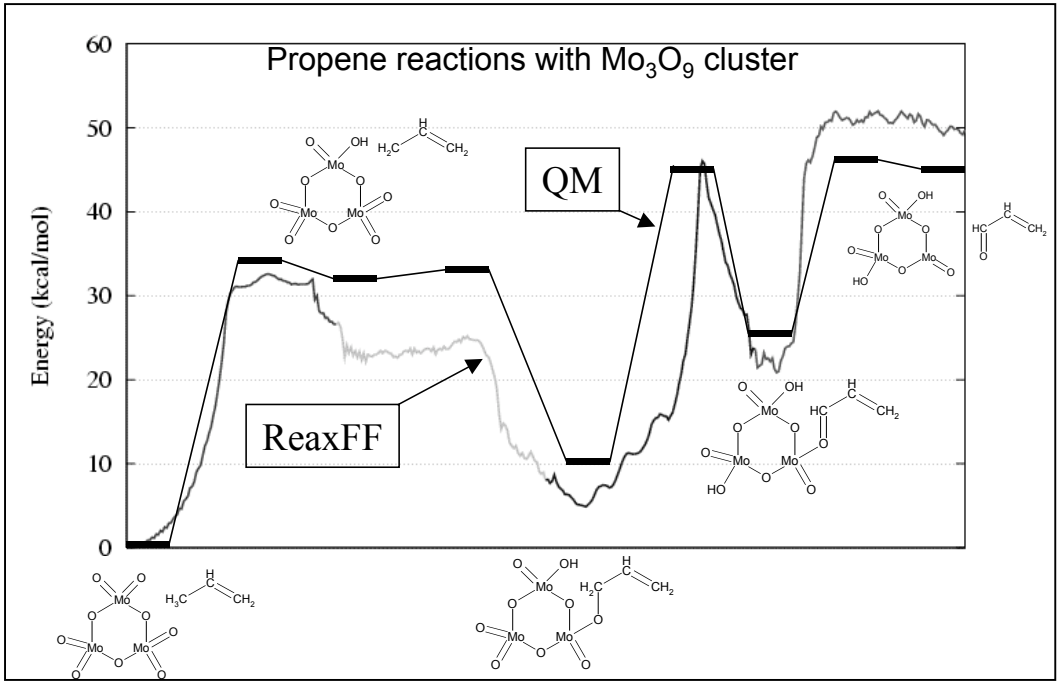
Angle strain

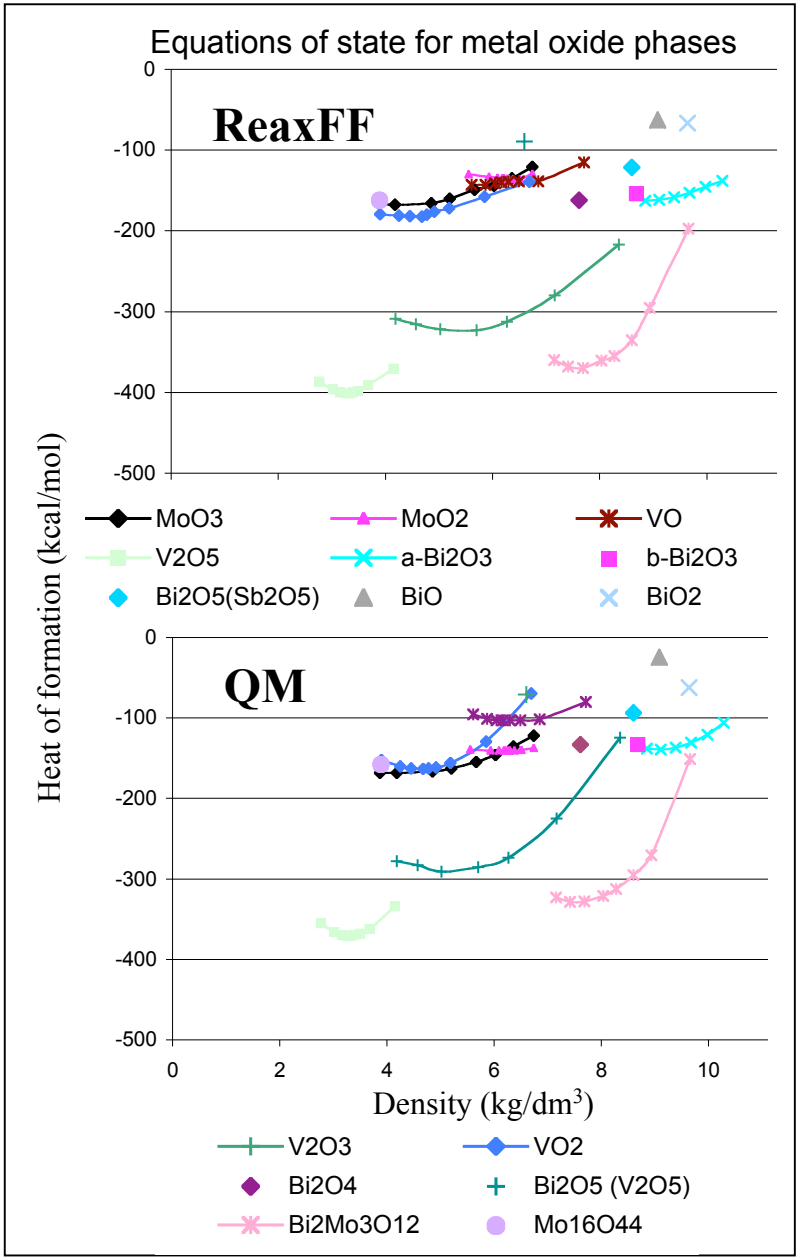


- total training set contains about 1700 compounds

Force field development: metal oxides

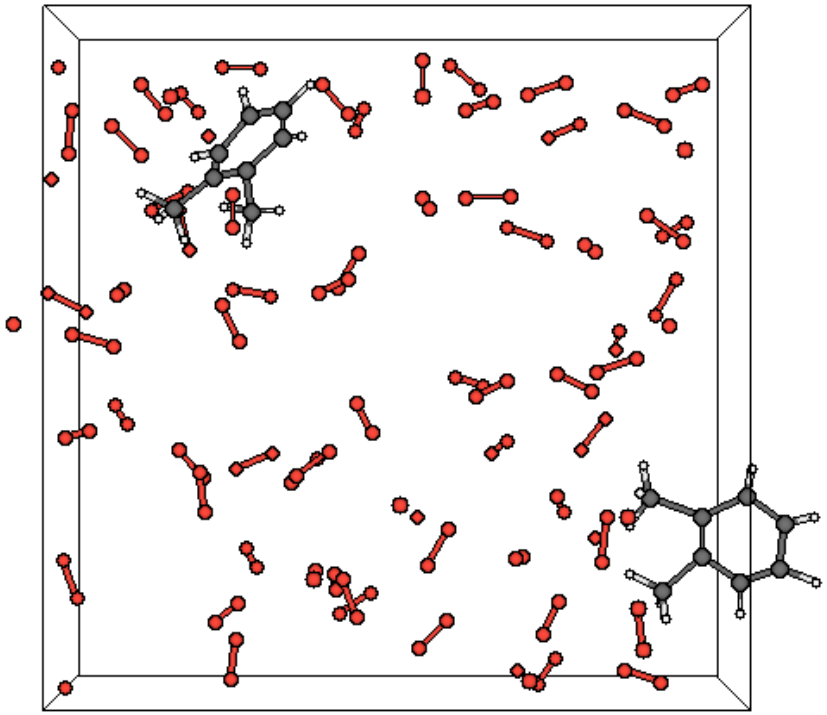




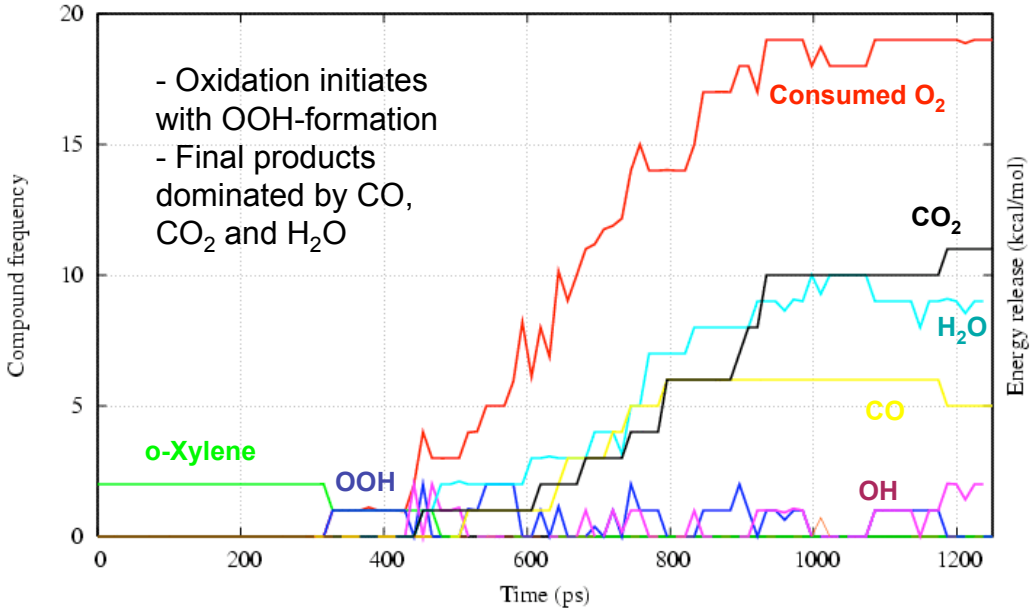


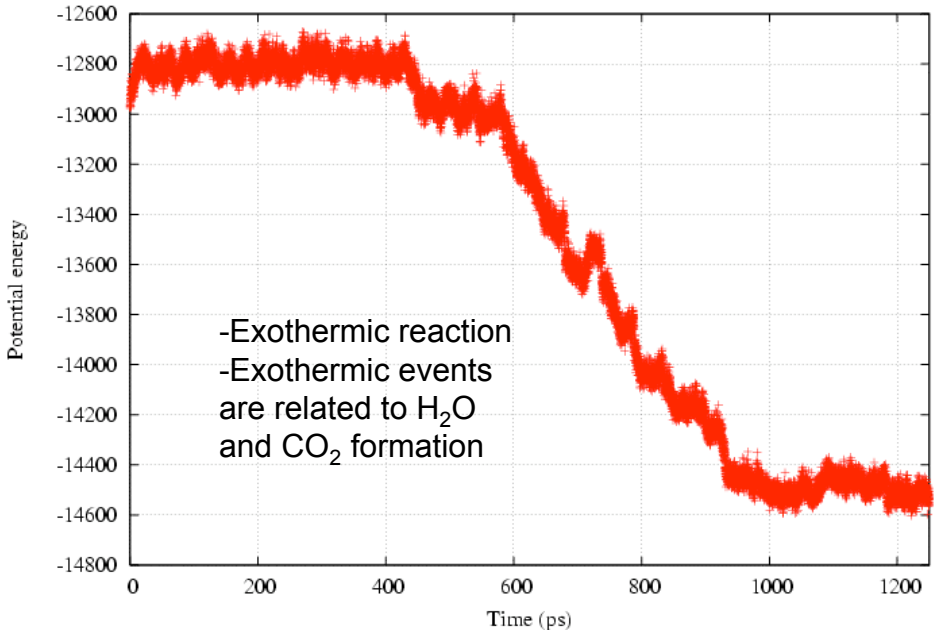
Goddard, van Duin, Chenoweth, Cheng, Pudar, Oxgaard, Merinov, Jang and Persson, Topics in Catalysis 2006

Test ReaxFF CHO-description: oxidation of o-xylene

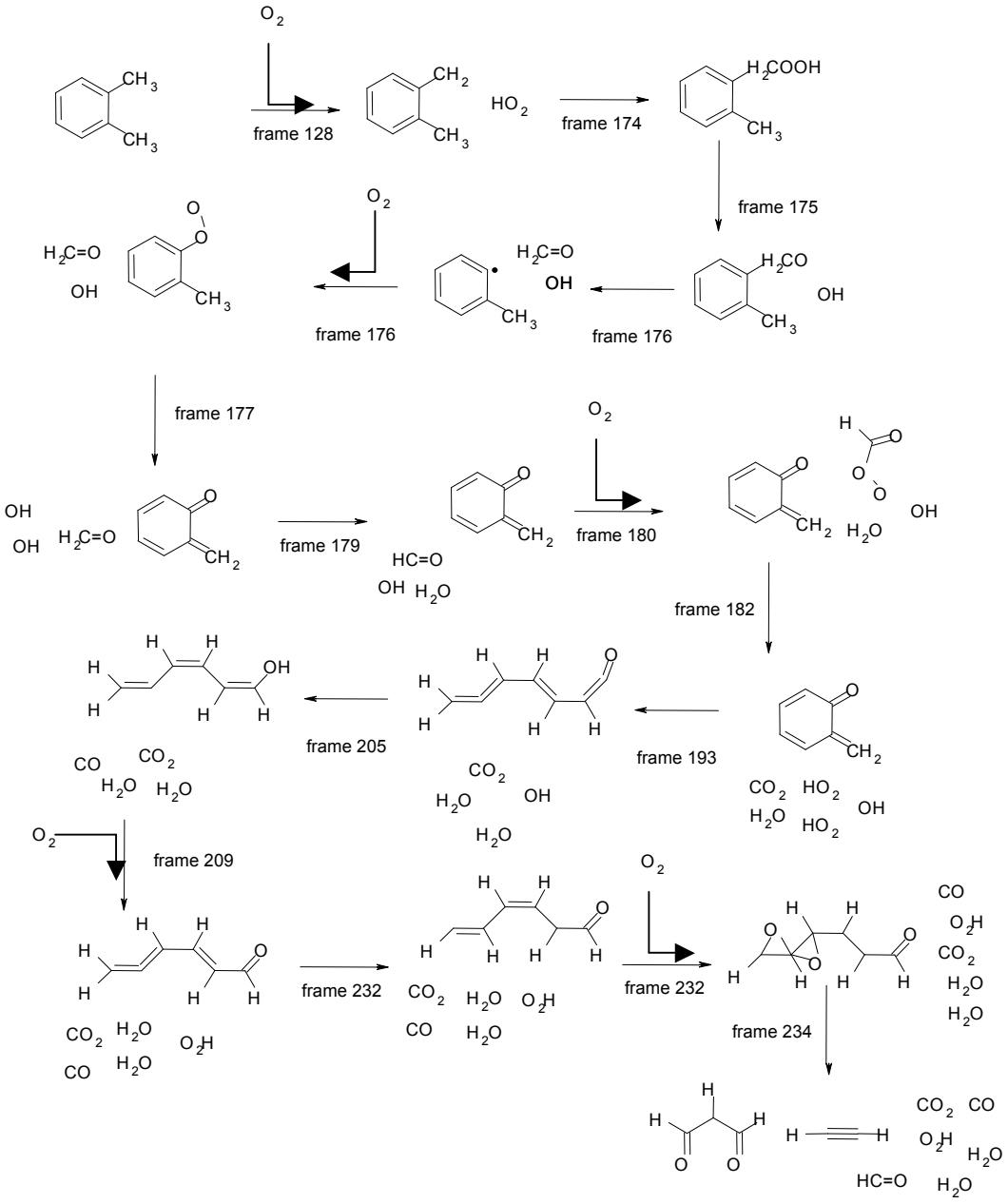


2 o-Xylene; 70 O_2 in 20x20x20 Angstrom box
ReaxFF NVT/MD at T=2500K





o-Xylene oxidation: Detailed reaction mechanism



- Reaction initiation with HO_2-formation

- Dehydrogenation occurs at methyl-groups, not at benzyl-hydrogens

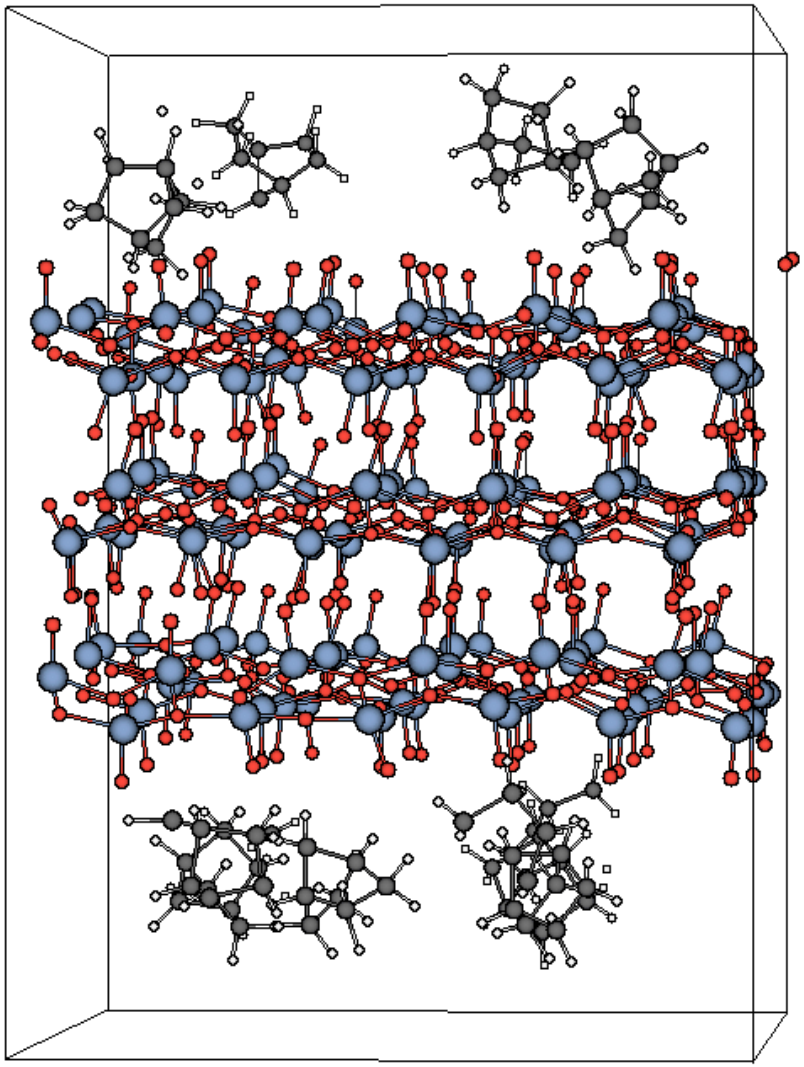
- Only after $H_2C=O$ is formed and dissociated the benzene ring gets oxidized

- Ring opens shortly after destruction of aromatic system

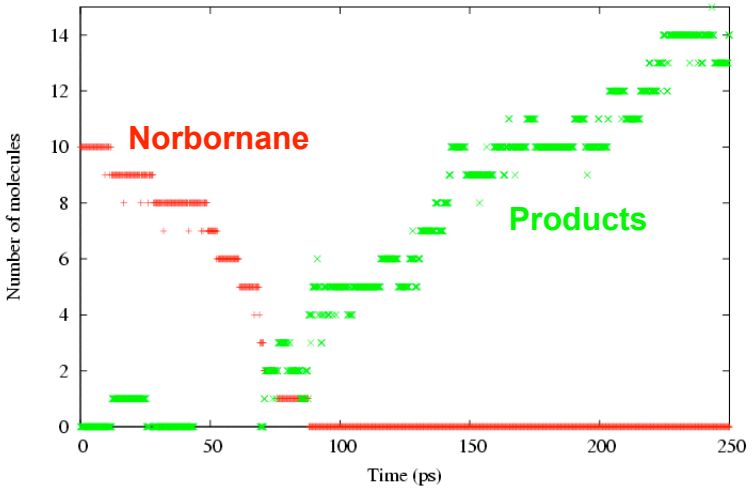
- Ring-opened structure reacts quickly with oxygen, forming CO_2, H_2O and CO

- ReaxFF gives sensible predictions that can be directly tested against QM

V_2O_5-catalyzed hydrocarbon oxidation



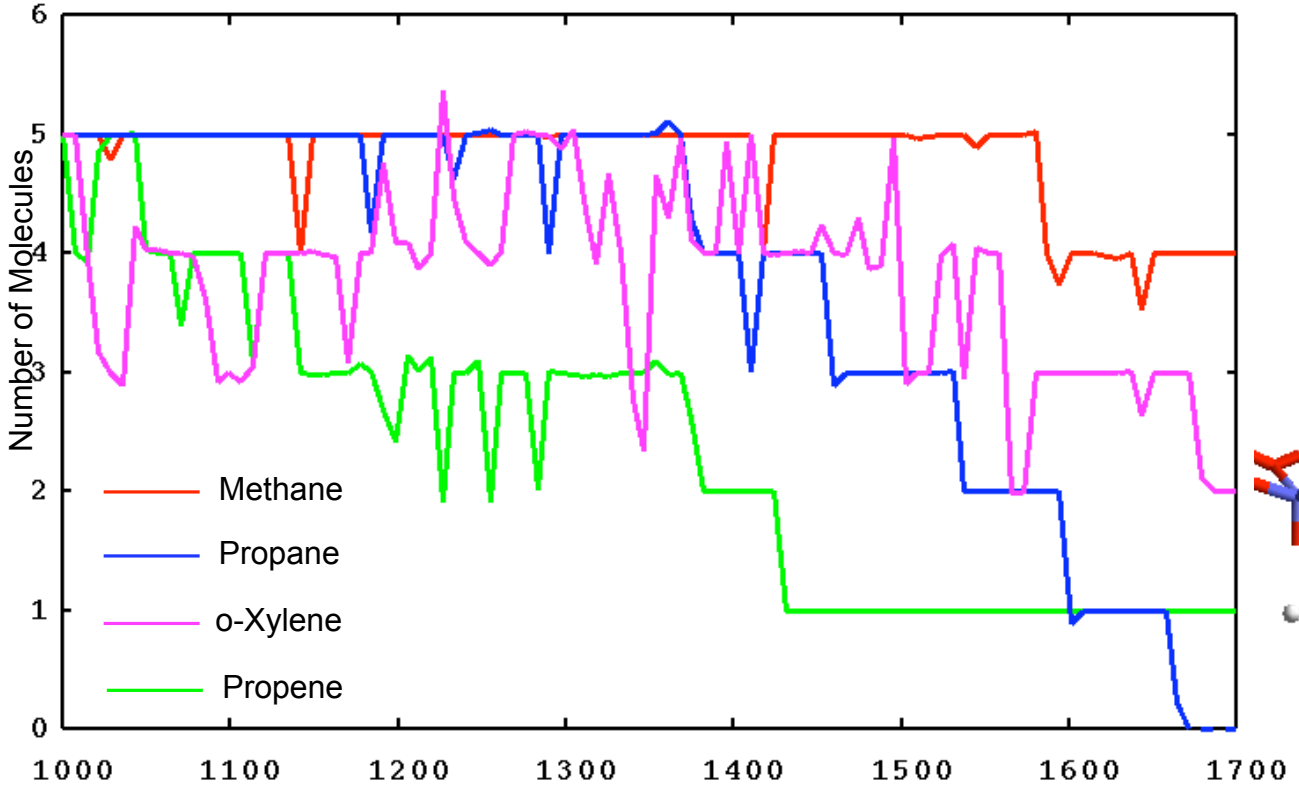
Norbornane/V_2O_5-system
NVT/MD at T=1600K

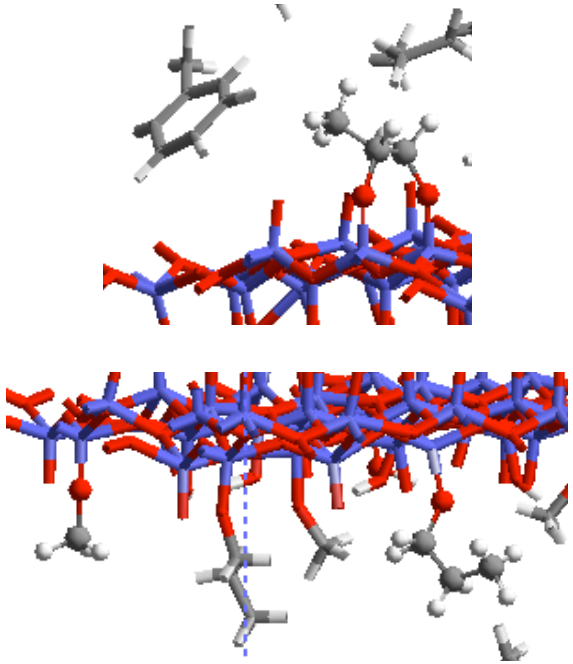


- Predict relative activity of various metal oxide phases
- Predict reaction rates for different hydrocarbons
- Predict kinetics as a function of temperature/pressure/composition
- Find active sites; check with QM

- Metal oxide slab (~600 atoms) kept at 500K and heatup hydrocarbons at 0.002K/fs for 125 ps
- Temperature control using Berendsen thermostat with 0.1 ps damping constant using a MD time step of 0.25fs

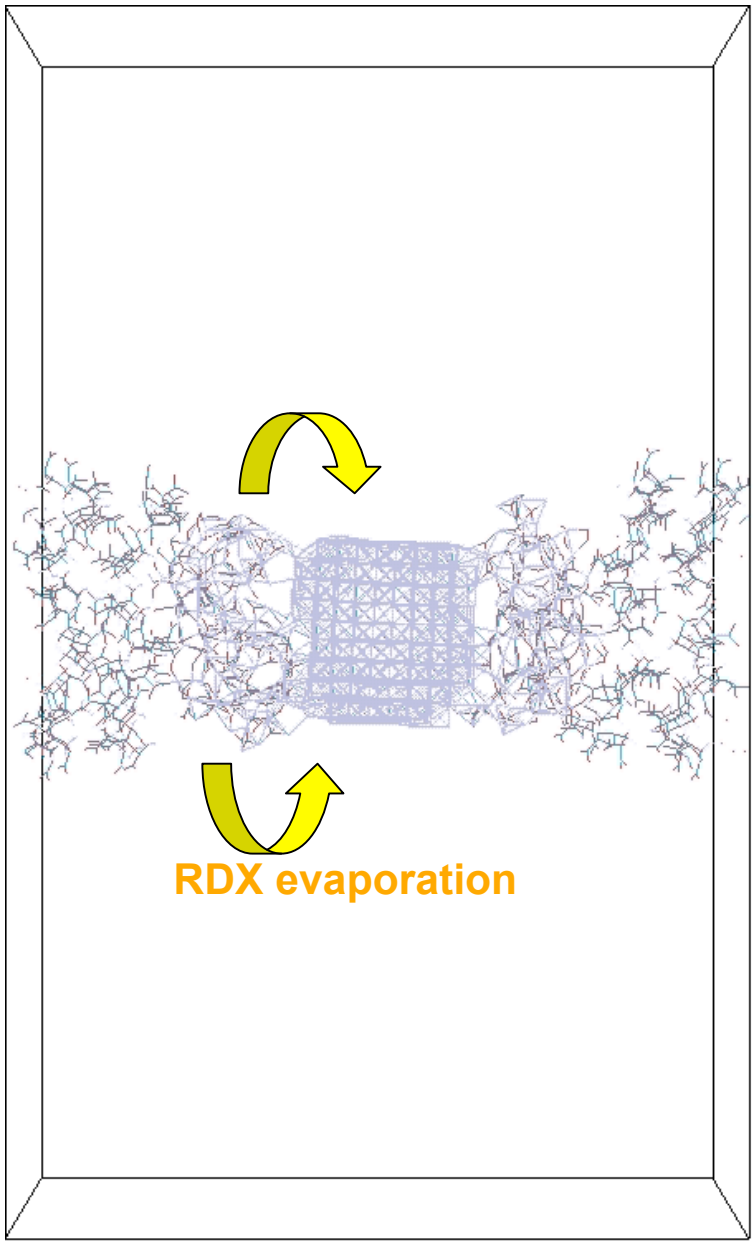
Selective Hydrocarbon Activation on V_2O_5 Surface

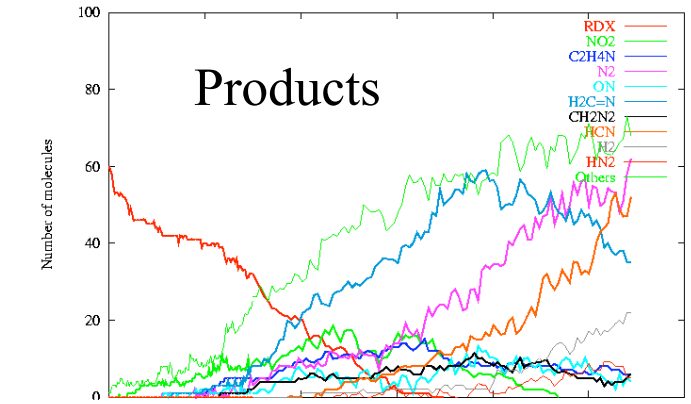




- **Propene reacts first and methane reacts last which is consistent with C-H bond strength**
- **C-H Bond Strength: Propene < o-Xylene < Propane < Methane**

Multicomponent combustion: gas/surface burning in a Al/Al_2O_3/nitramine system

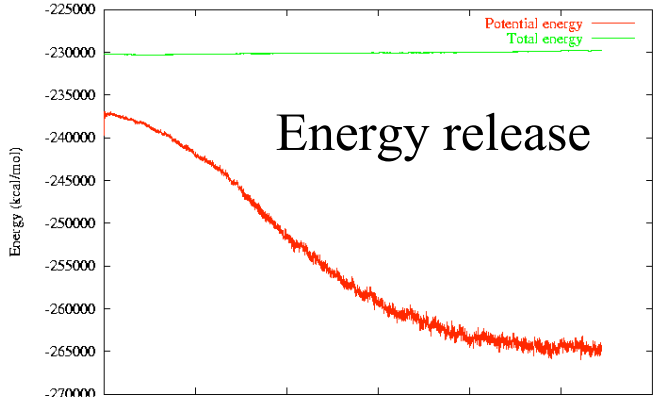




-Main products: N_2, HCN, $H_2C=N$

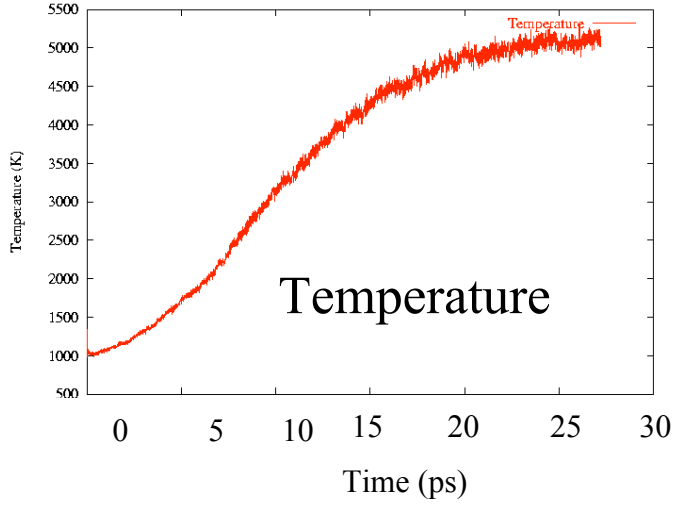
- NO_2 is main intermediate

- All oxygen ends in Al-phase

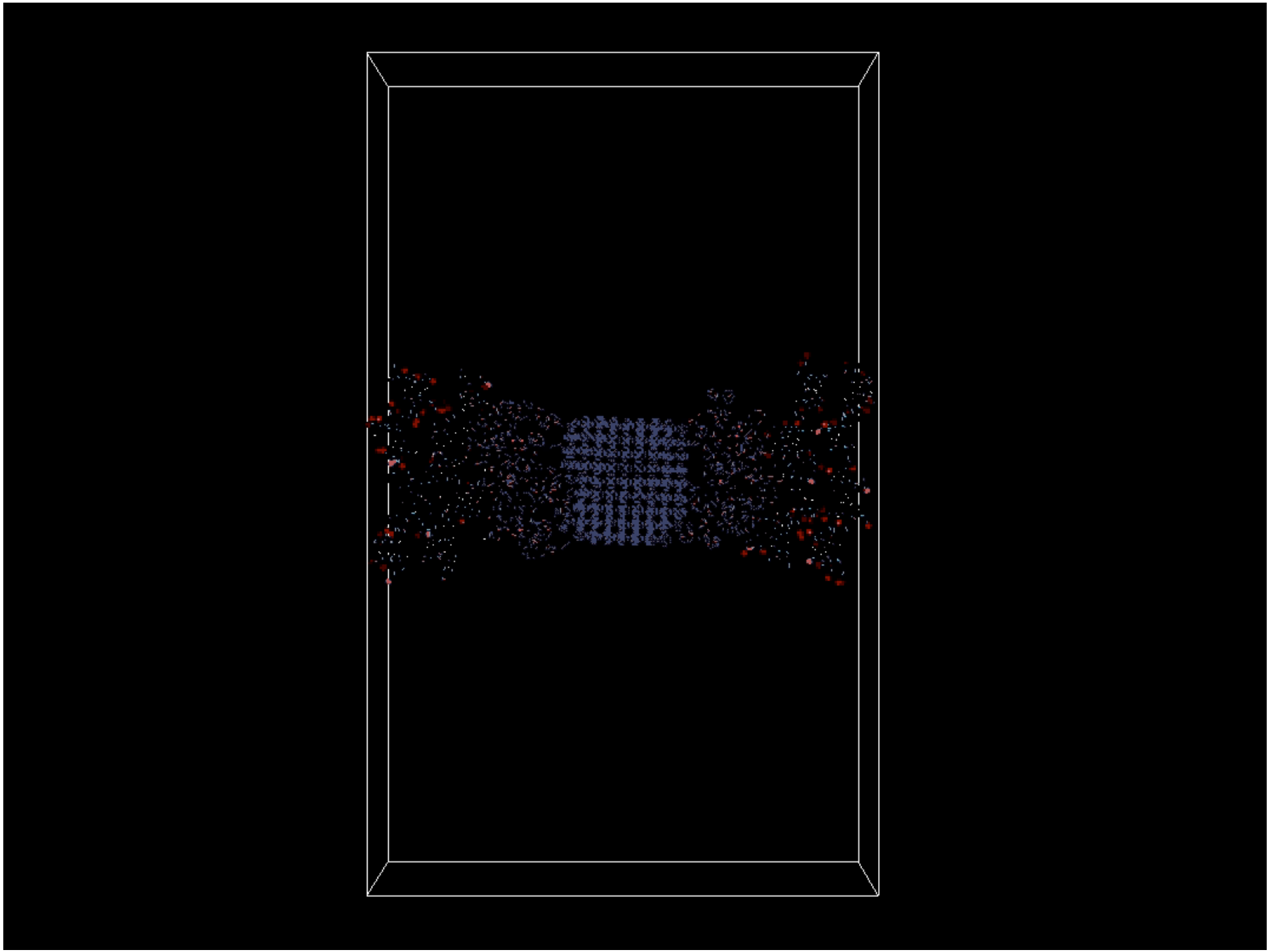


- Good energy conservation during NVE simulation

- Energy release stops at t=25 ps.



- Final temperature around 5250K



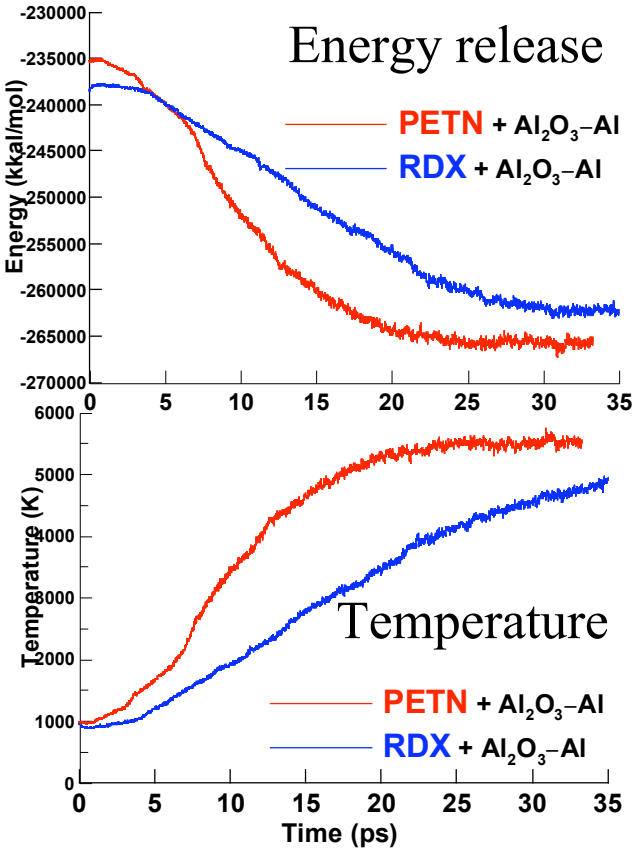
Comparison of ISP for different systems

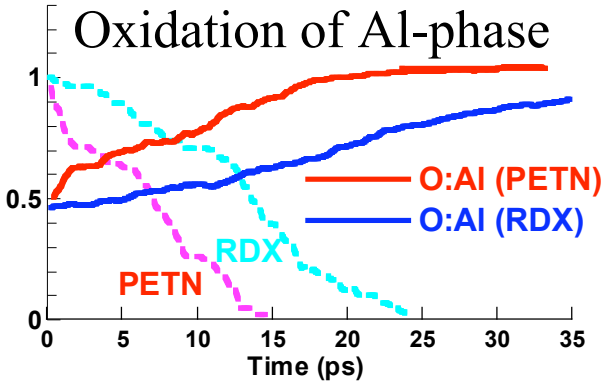
	Mass kg/mol	Energy kcal/mol	T_{final}	$I_{sp,max}$
PETN+Al/Al_2O_3	**37.52**	**30527**	**5520 K**	**267 s**
RDX+Al/Al_2O_3	**37.25**	**27474**	**5113 K**	**254 s**

Initial compositions (PETN has better oxygen balance):

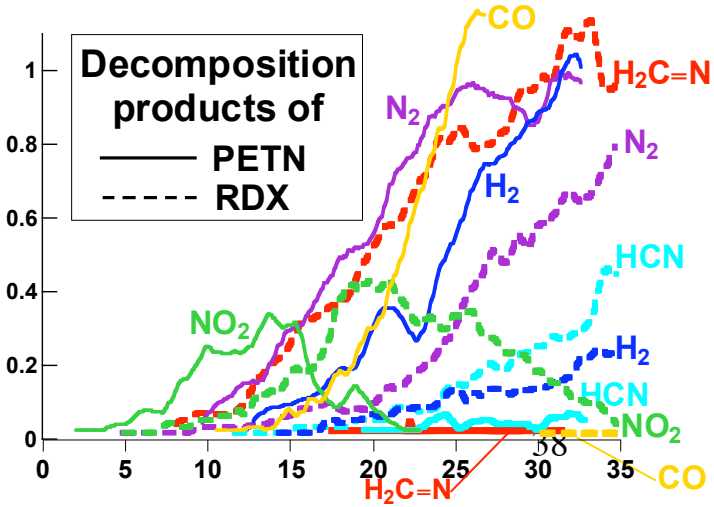
PETN: $43\times C_5H_8O_{12}N_4 + Al_{462}/Al_{238}O_{326}$ **RDX:** $58\times C_3H_6O_6N_6 + Al_{462}/Al_{238}O_{326}$

Final compositions: **PETN:** $Al_{665}O_{704}N_{36}C_{16}H_{85}$ **RDX:** $Al_{671}O_{623}N_{72}C_8H_{38}$





- Initial temperature T_0=1000K for both systems
- PETN provides more oxygen for Al-phase oxidation
- Rate of oxidation of Al-phase is higher for PETN-based propellant



- Rate of PETN decomposition is higher than of RDX.
- PETN exhibits faster dissociation of NO_2-fragments which initiate early burning of Al-metal surface.
- PETN provides higher oxidation rate of Al-phase and larger final stoichiometry (~13%) of the oxidized Al in comparison with RDX.
- Decomposition products are also different: PETN-composite does produce very little $H_2CN{=}N$, HCN, but more N_2, CO, and H_2

- ReaxFF: background, rules and current development status
- Stress-induced crack propagation
    - Integration of ReaxFF in a multi-paradigm computational framework (CMDF)
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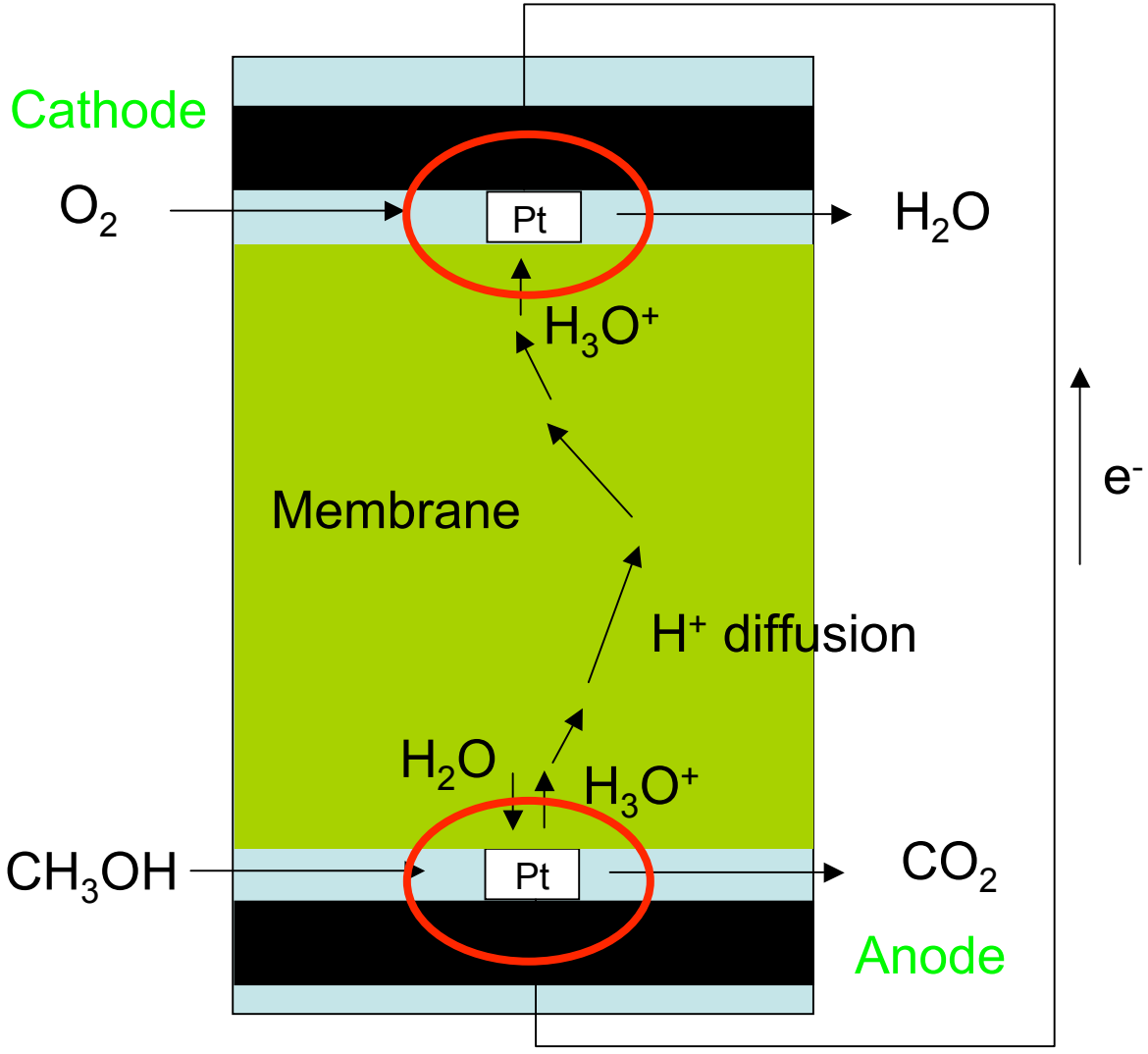
    - Methanol conversion on Pt[111]
    - Ni/Cu/Co catalyzed nanotube formation
    - H_2 dissociation on a Ni_{309}-particle

Fuel cells: anode/cathode catalysis

Collaborators: Sang Soo Han, Seung Soon Han, Valeria Molinero, Yun Hee Yang (GIST, Korea), Timo Jacob (FHI), Boris Merinov and Bill Goddard



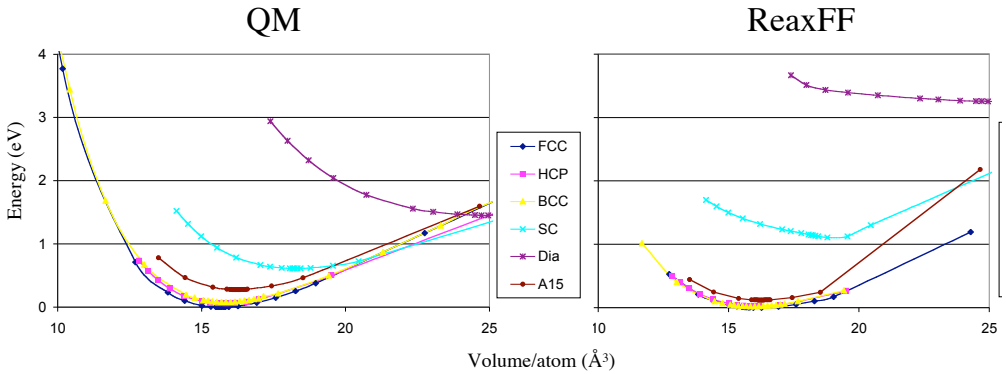
Direct methanol fuel cell

- Aim: perform atomistic scale reactive dynamics simulation on a realistic model of the entire fuel cell
- Complicated chemistry, need relatively large system to capture all aspects
- Use QM-data on isolated systems to parameterize ReaxFF, then use ReaxFF on full system

Force field development

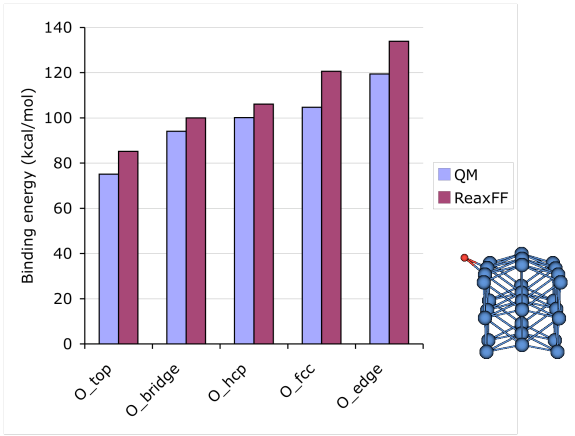
1. Bulk metal, metal clusters and metal surfaces

Equations of state for bulk metal phases

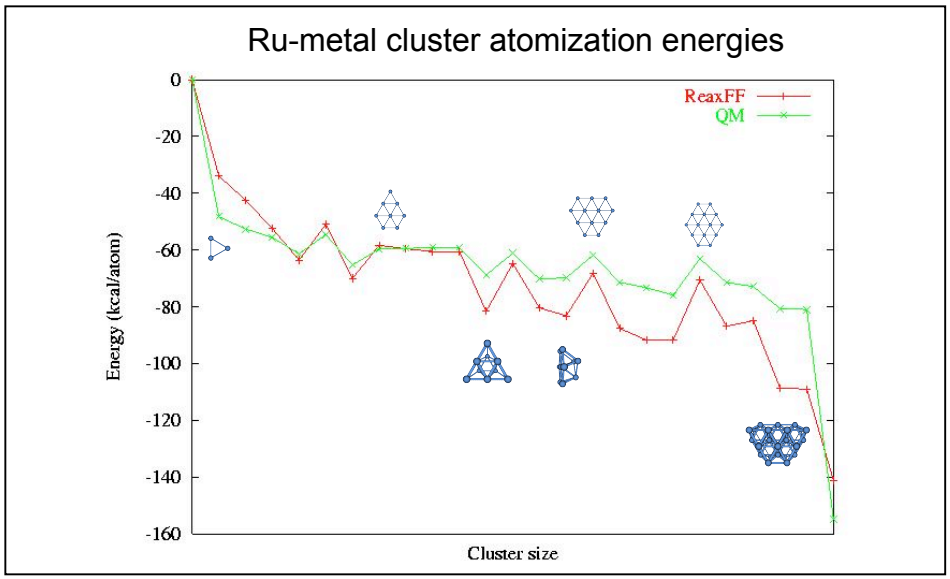


Pt-bulk phases

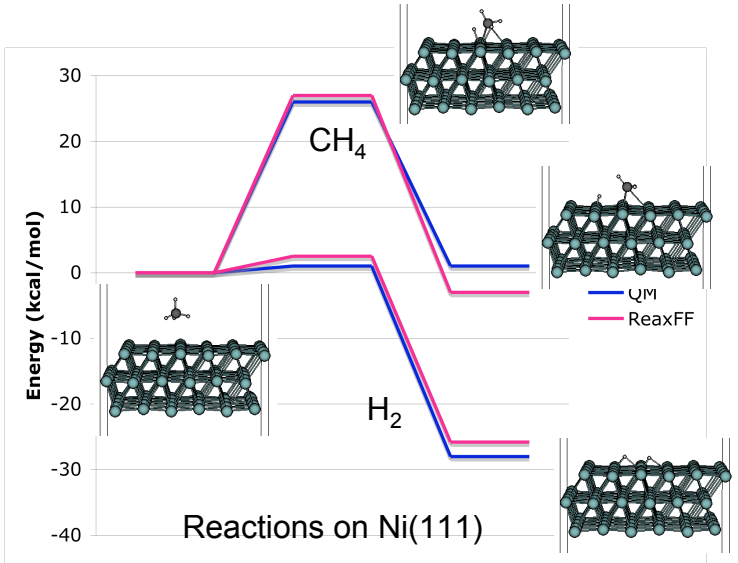
Oxygen binding to Ru_{28}-clusters



Ru-metal cluster atomization energies

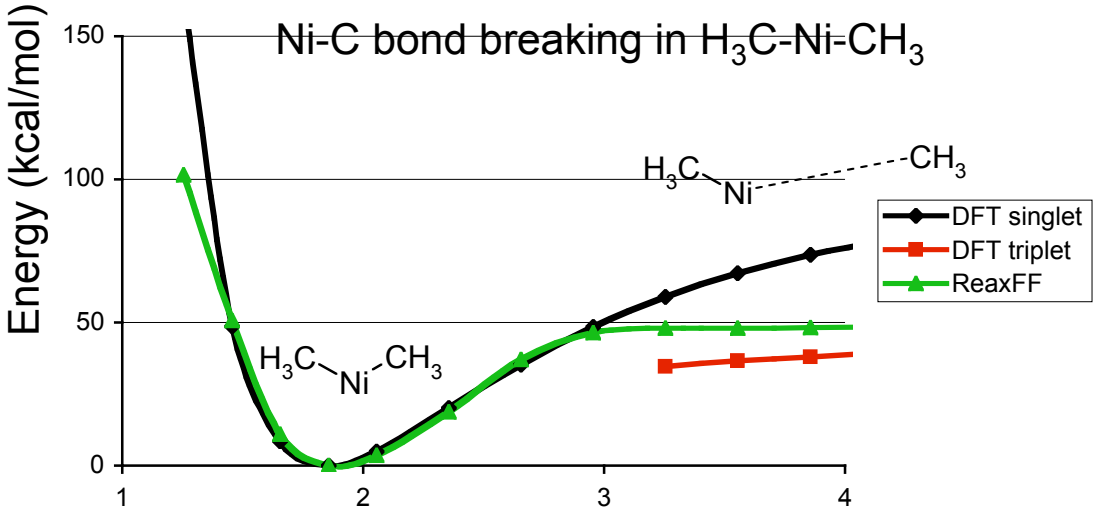


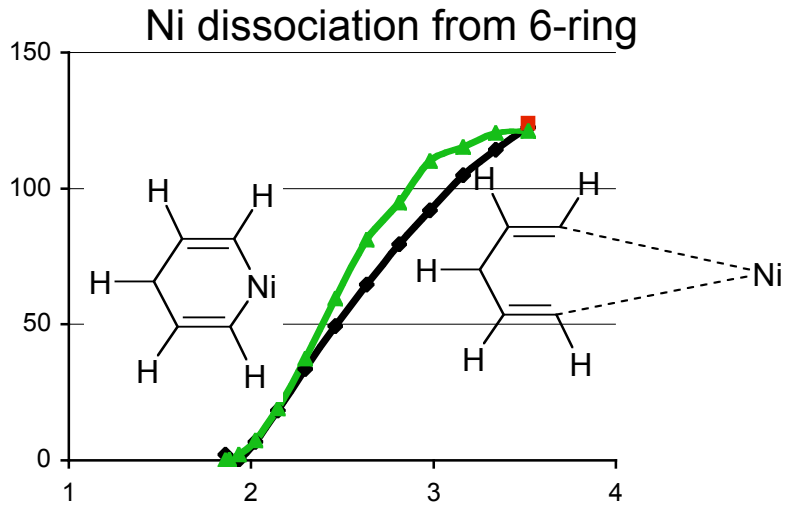
Barriers for reactions on metal surfaces

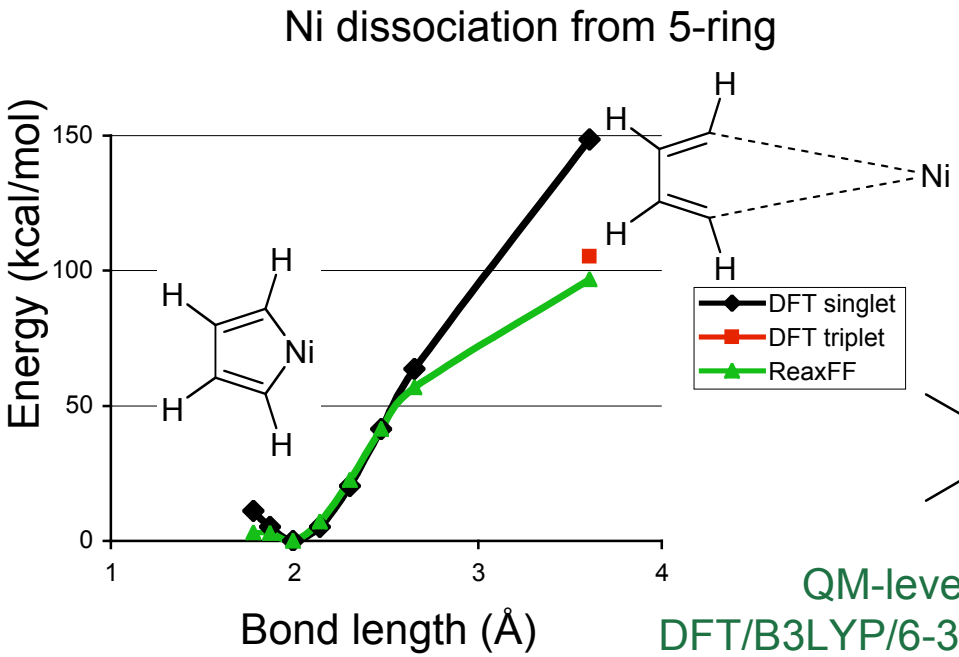


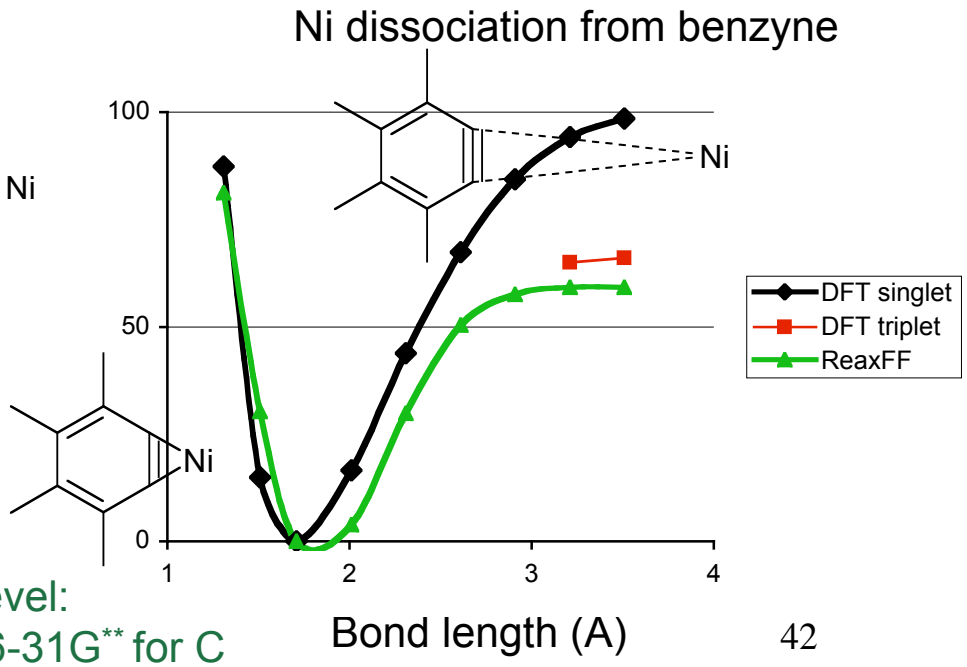
- ReaxFF parameters available for Na, Mg, Ca, Ba, Ti, V, Co, Ni, Cu, Al, Y, Zr, Mo, Te, Ba, Ru, Pt and Bi-metals

2. Ni/hydrocarbon clusters



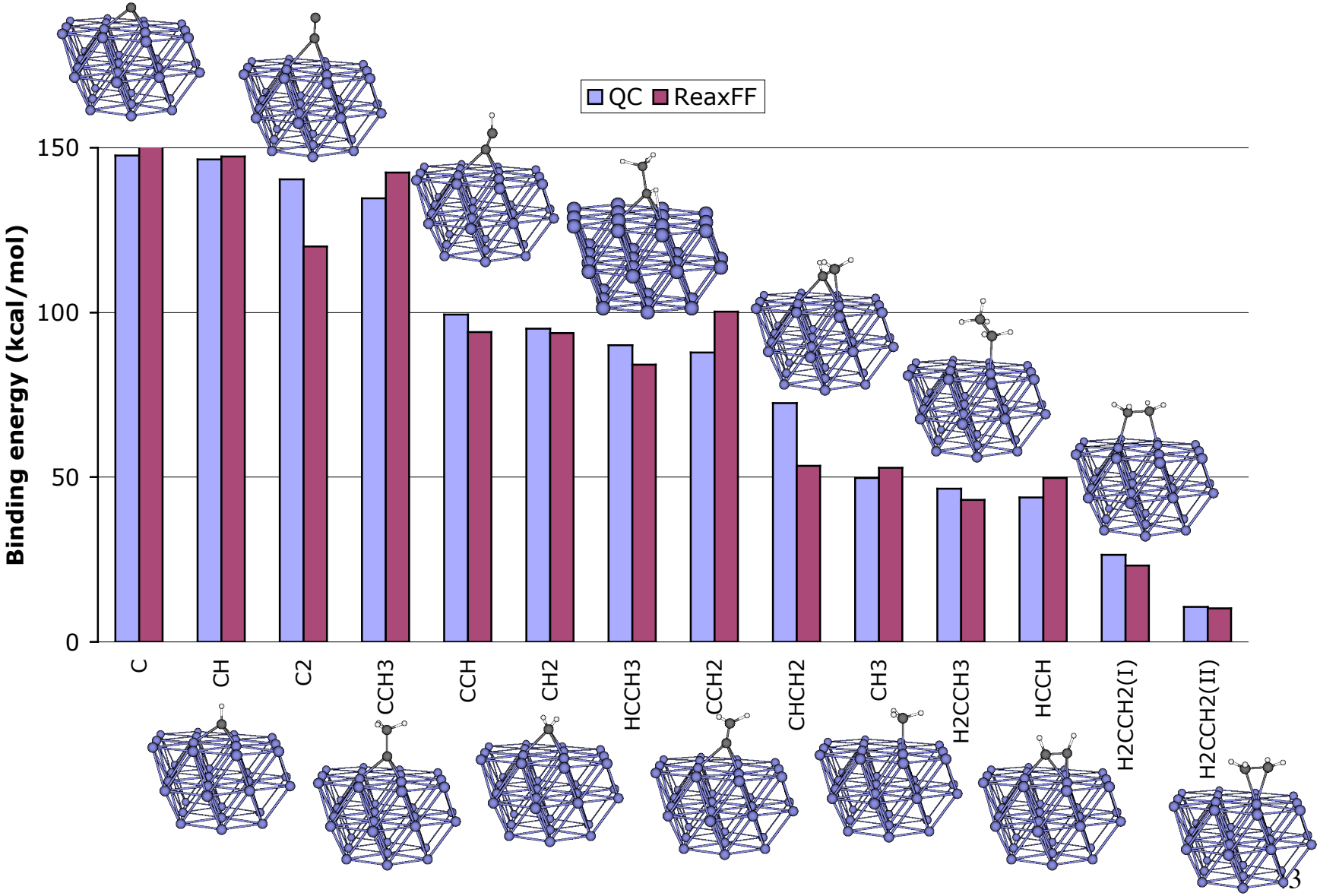




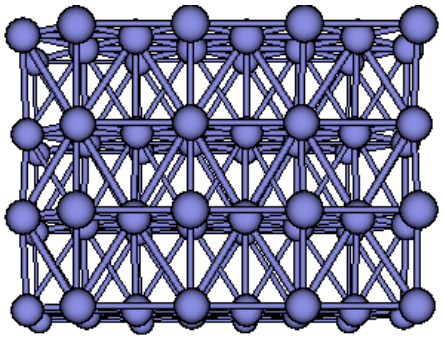


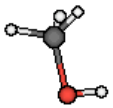
QM-level:
DFT/B3LYP/6-31G** for C
DFT/B3LYP/LACVP** for Ni

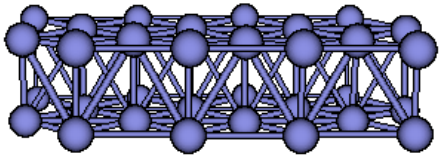
3. Hydrocarbon binding to Pt_{35}-clusters

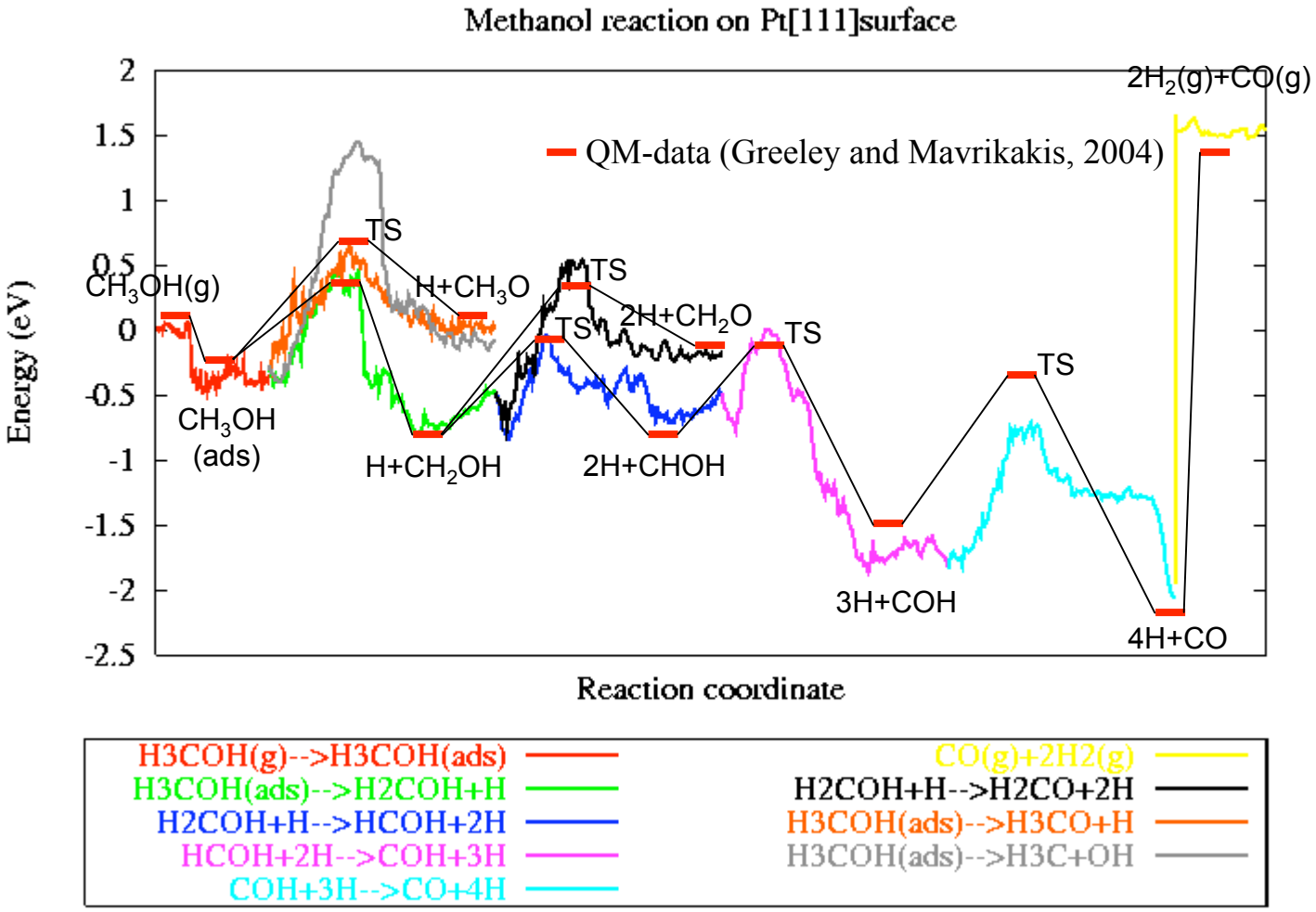


4. Reaction pathways







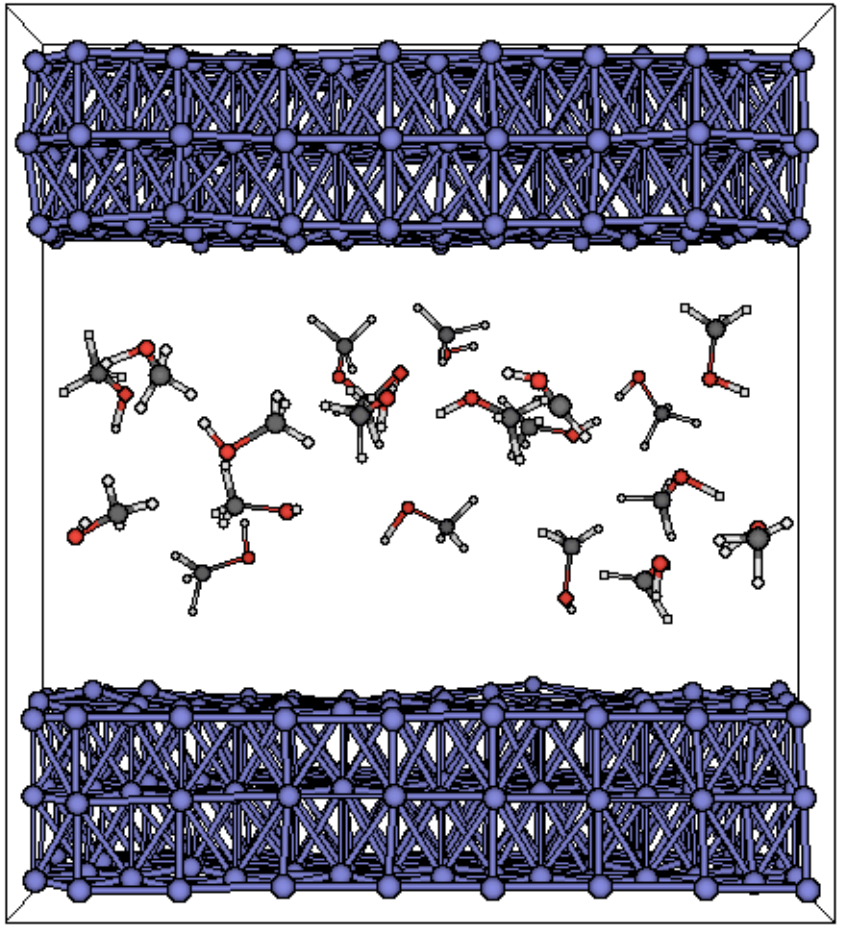


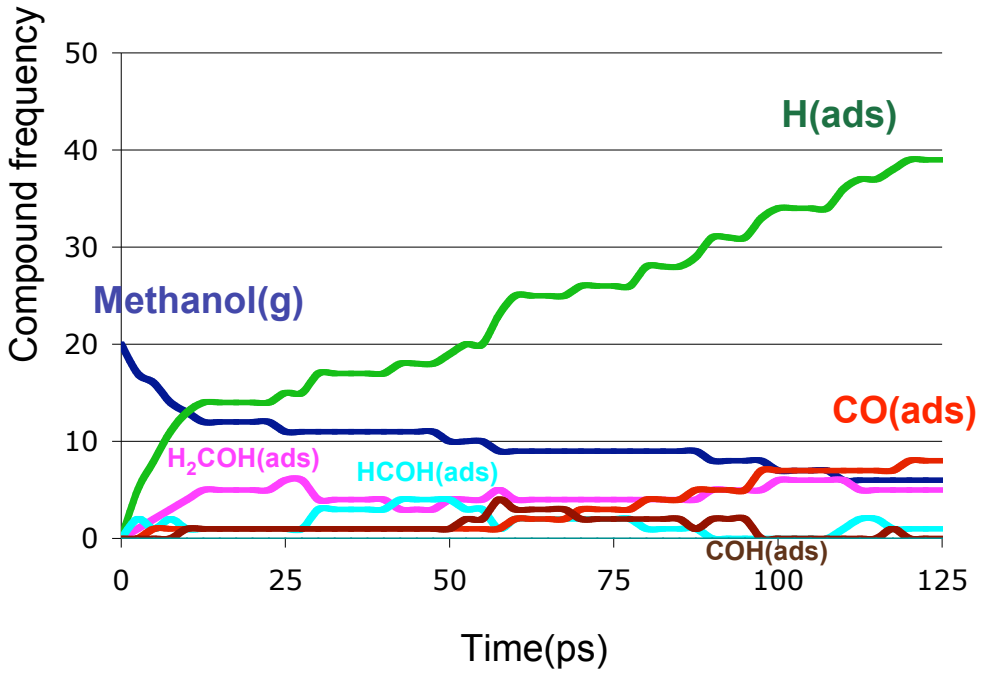
- Excellent agreement between ReaxFF and QM for entire reaction path

Applications of the Ni/Pt ReaxFF potentials

1. Methanol conversion on Pt[111]-surface

MD-simulation at T=1250K on methanol/Pt[111]



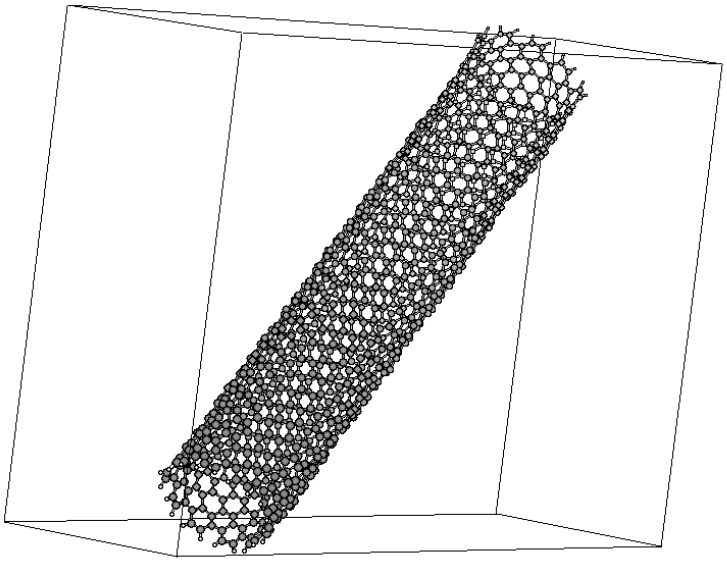


- Methanol dissociates on Pt-surface, generating adsorbed hydrogen
- CO accumulates on surface (poisoning)
- ReaxFF descriptions for Ti, Mo, V, Bi, Ru, Ni under development

2. Ni/Co/Cu catalyzed nanotube formation

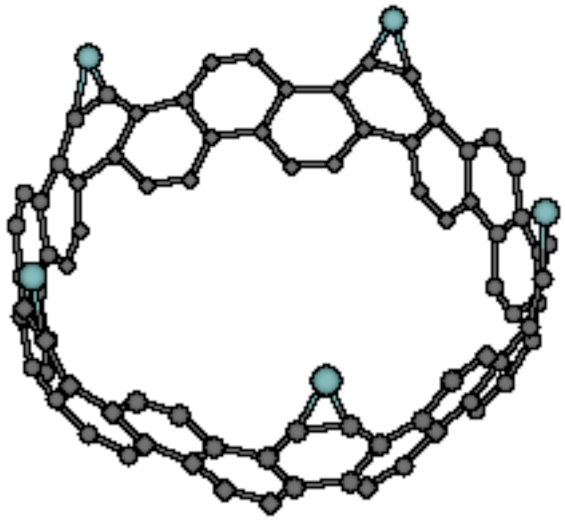
Collaborators: Si-ping Han, Kevin Nielson, Weiqiao Deng, Jonas Oxgaard, Mark Lusk (CSM) and Bill Goddard

Carbon source $\xrightarrow[\text{metal catalyst}]{\text{high T}}$



Nanotube

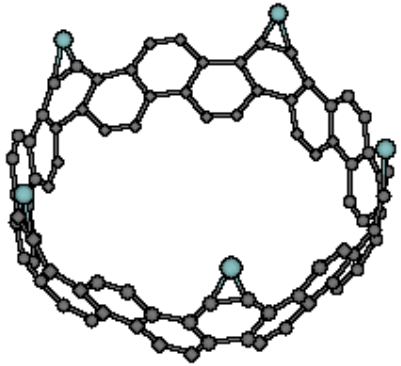
- Synthesis mechanism not clear
- Metal influences reaction product (single, double wall, nanotube diameter, nanotube/buckyball ratio)



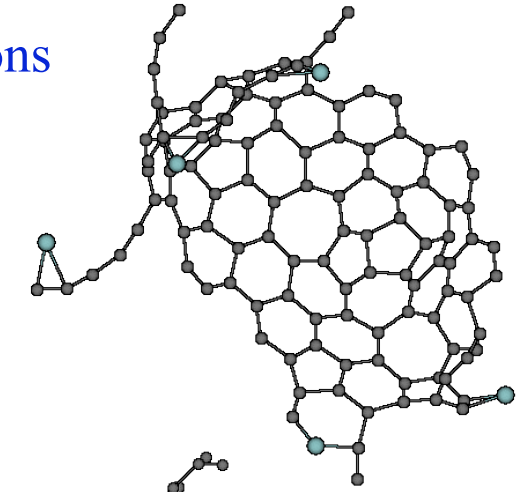
- Ni-atoms can grab C_2-monomers and fuse them as new 6-membered rings

- Start configuration: 20 C_6-rings, 5 metal atoms on edge
- NVT simulation at 1500K
- Add C_2-molecule every 100,000 iterations

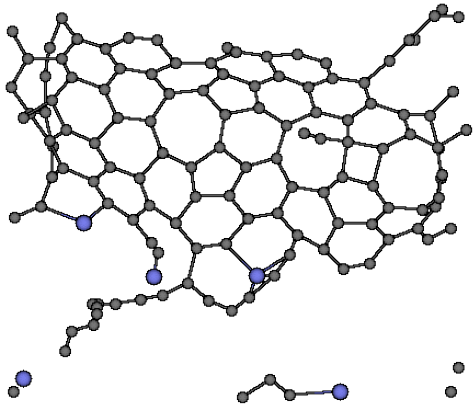
Results after 2,000,000 iterations



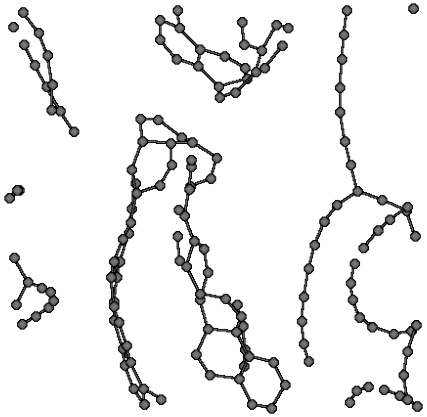
Metal=Ni



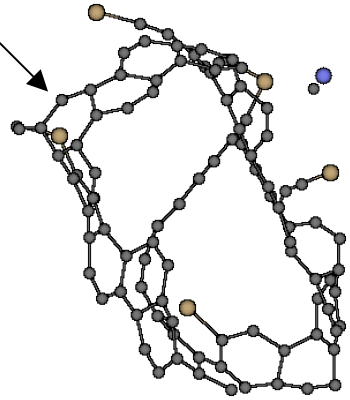
Metal=Co



No metal



Metal=Cu

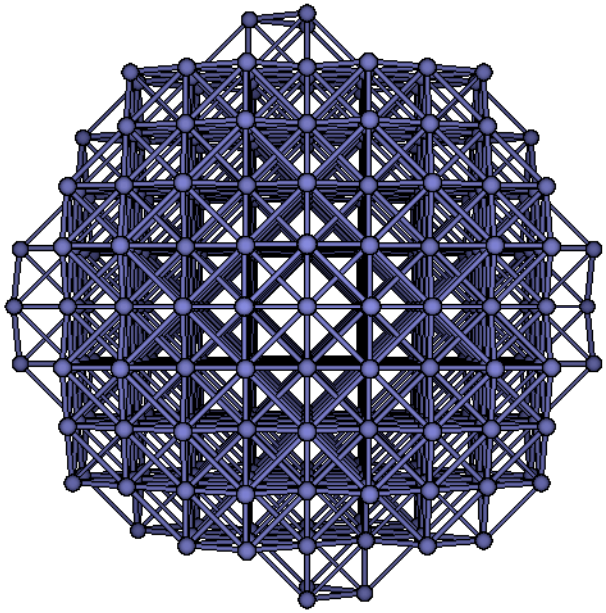


-Ni and Co lead to greatly enhanced ring formation. Cu is far less active.

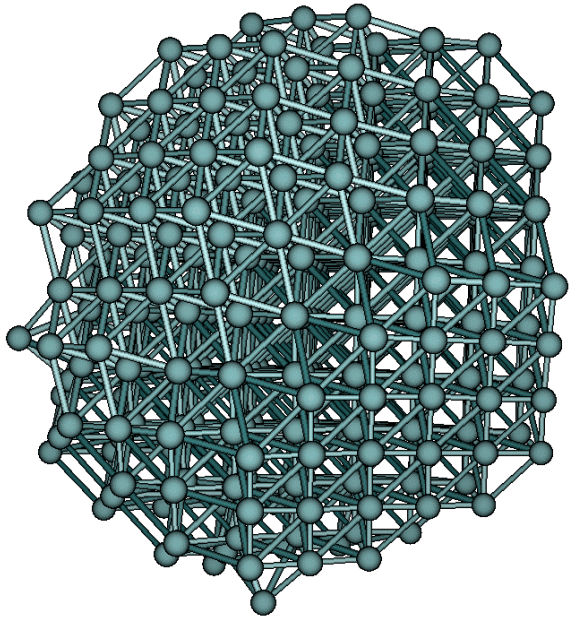
Nielson et al., JPC-A 2005

3. H_2 dissociation on a Ni_{309}-particle

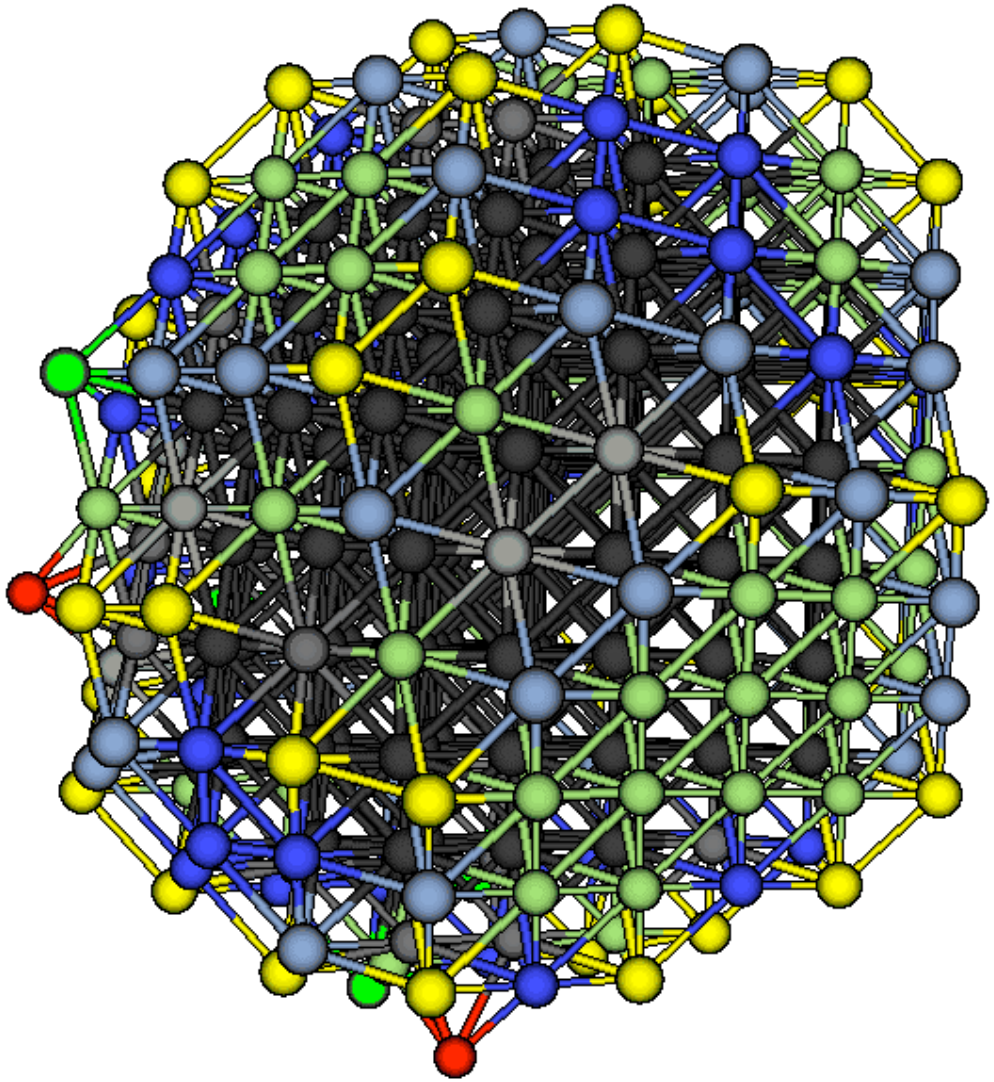
Preparation of the Ni_{309}-particle



Initial configuration: sphere in fcc-configuration
- Heat up to 1600K to melt surface
- Cool down to 300K to form surface facets
- [111] surface dominate
- Core retains fcc-configuration



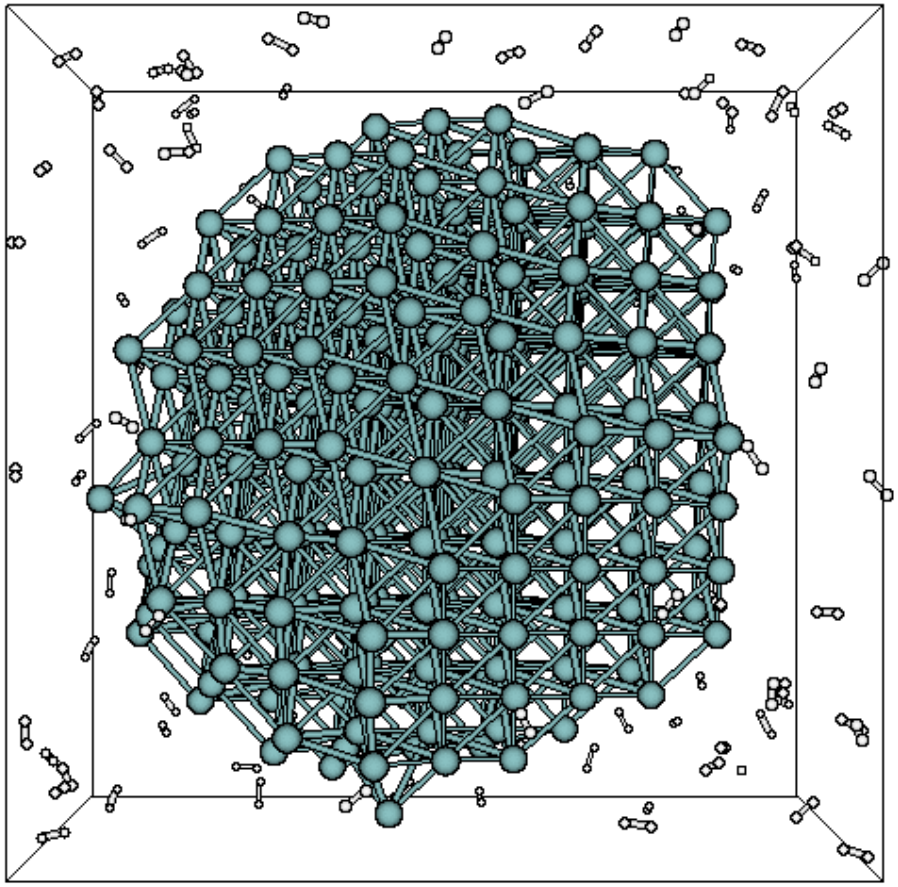
Analysis of the Ni_{309}-particle

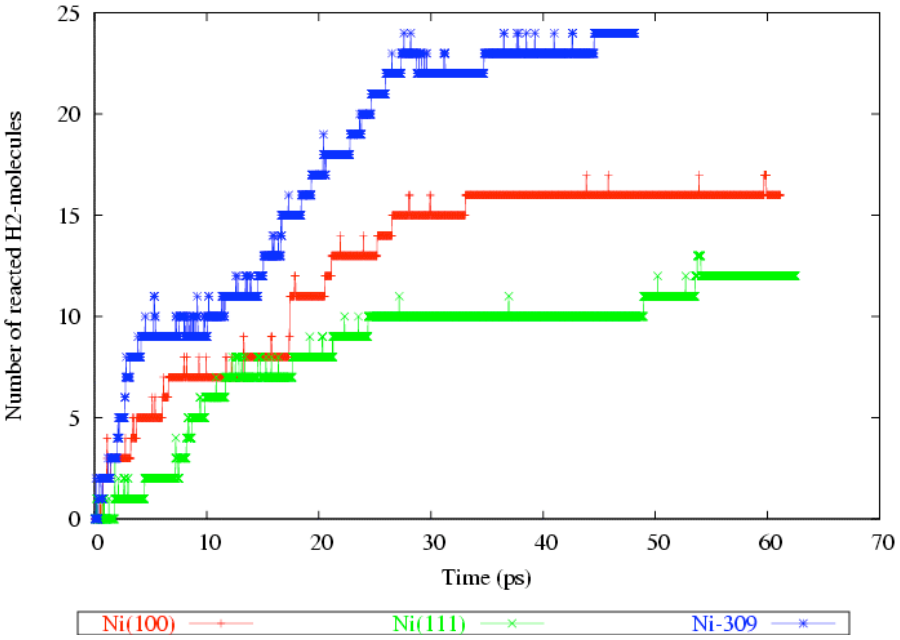


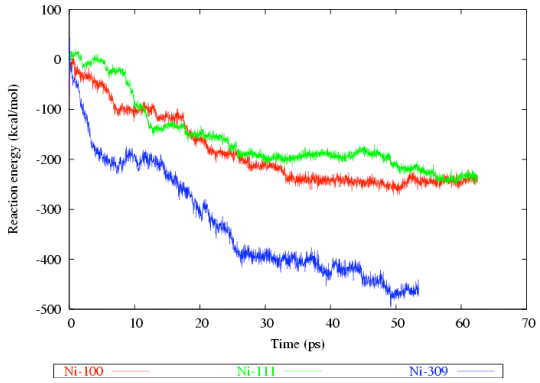
12 neighbours (fcc):	133 atoms
11 neighbours:	17 atoms
10 neighbours:	8 atoms
9 neighbours (111 facet):	41 atoms
8 neighbours (100 facet):	33 atoms
7 neighbours:	34 atoms
6 neighbours (edge):	37 atoms
5 neighbours (adatom):	4 atoms
4 neighbours (adatom):	2 atoms

- Surface dominated by 111-facets and related edges

Reaction with H_2 at T=300K

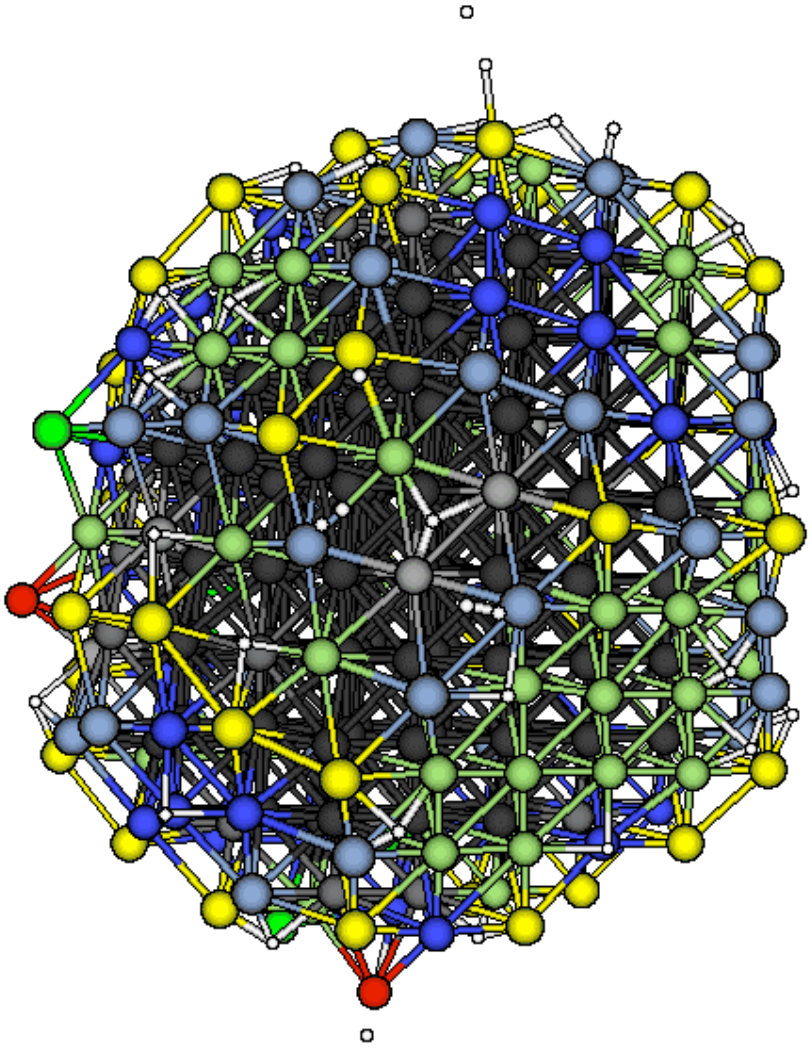






- Ni_{309} reacts faster than Ni(100) and Ni(111)-surfaces
- Ni(100)- surface reacts faster than Ni(111)-surface
- H_2-dissociation stops when surfaces are saturated; no formation of subsurface hydrogen species

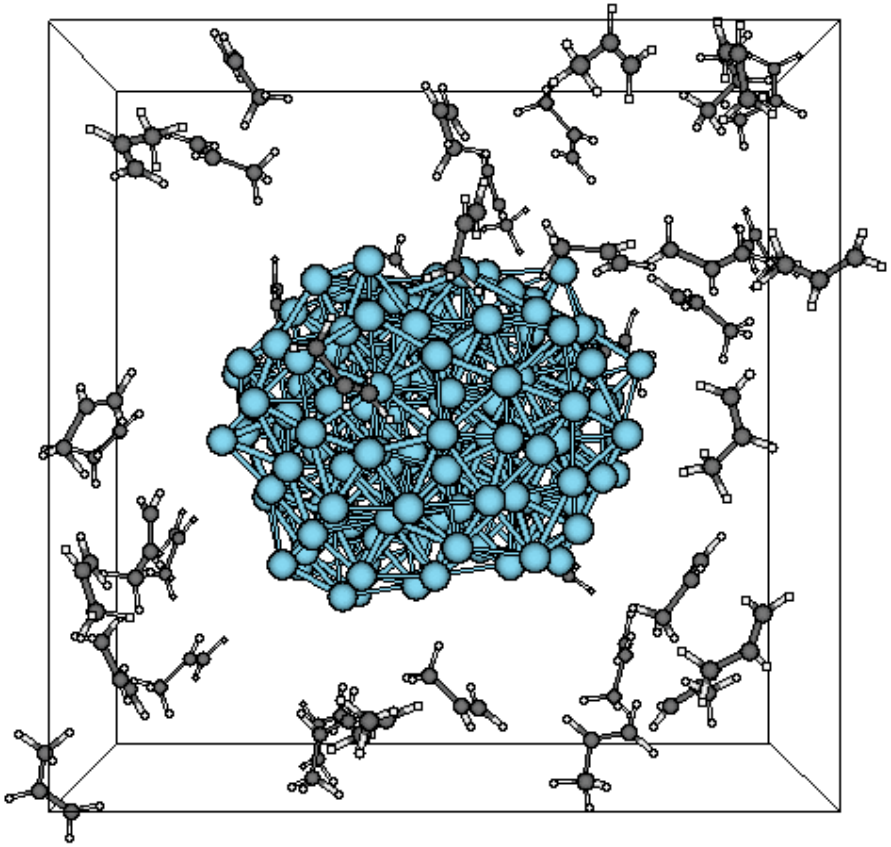
Analysis of hydrogen location



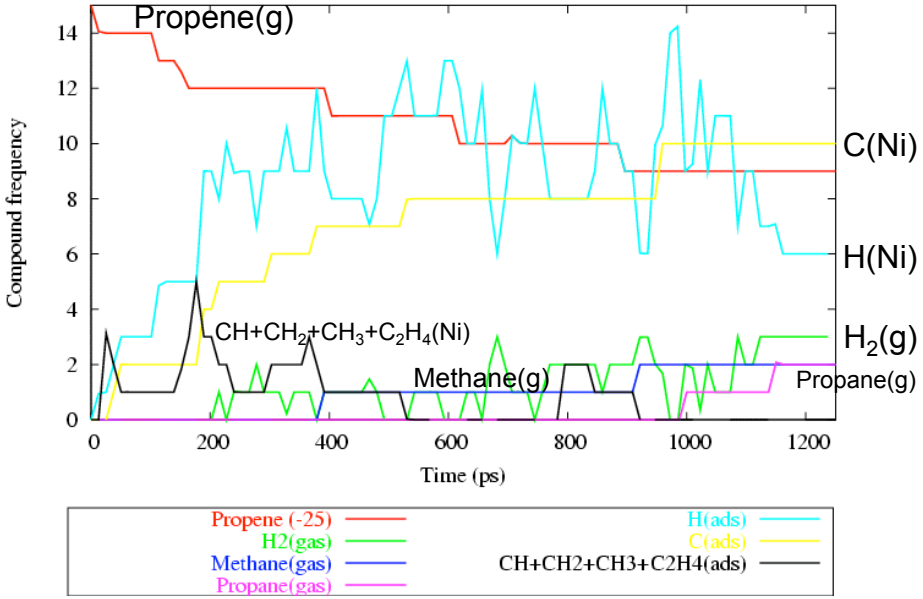
			% coverage
12 neighbours (fcc):	133 atoms	0 H	0%
11 neighbours:	17 atoms	9 H	53%
10 neighbours:	8 atoms	6 H	75%
9 neighbours (111 facet):	41 atoms	31 H	76%
8 neighbours (100 facet):	33 atoms	14 H	42%
7 neighbours:	34 atoms	12 H	35%
6 neighbours (edge):	37 atoms	12 H	32%
5 neighbours (adatom):	4 atoms	1 H	25%
4 neighbours (adatom):	2 atoms	0 H	0%

- Hydrogen accumulates on [111] facets, preferably around [111] edge sites
- Low-coordination Ni-atoms help dissociating H_2 but do not make stable Ni-H bonds; H diffuses on to [111] facets

Hydrocarbon conversion on Ni-particle



- Initial configuration: Ni_{147}-particle; 30 propene
- Temperature: 1500K
- Box size: 25x25x25 Angstrom

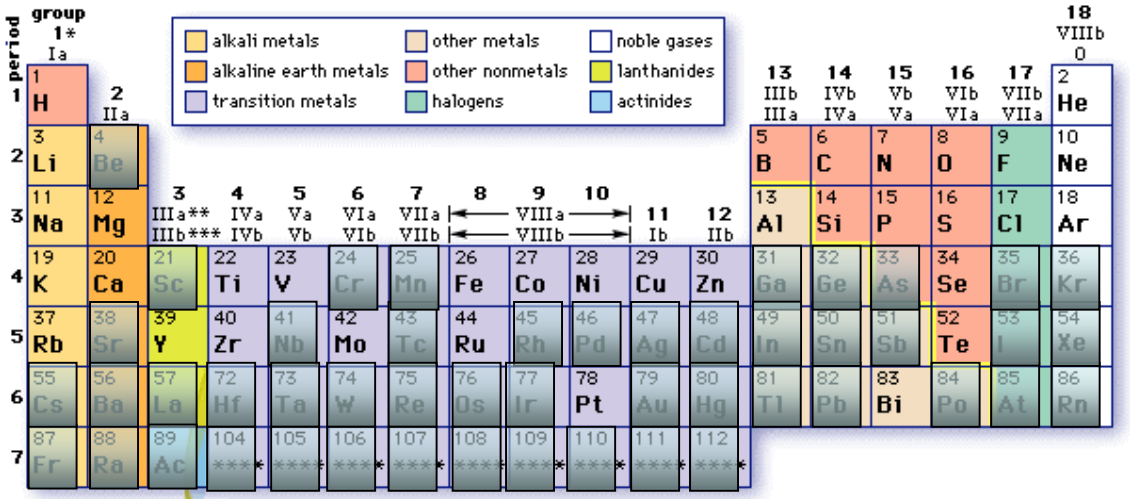


- Ni catalyzes C-H bond breaking in propene
- Carbon accumulates in Ni-cluster
- Hydrogen equilibrates with gas-phase H_2
- Relatively slow reaction (compared with H_2)
- C(ads) may eventually form CNT-like structures
- No surface-facets due to high temperature

Conclusions

- ReaxFF has proven to be transferable to a wide range of materials and can handle both complex chemistry and chemical diversity. Specifically, ReaxFF can describe covalent, metallic and ionic materials and interactions between these material types.

- The low computational cost of ReaxFF (compared to QM) makes the method suitable for simulating reaction dynamics for large (>> 1000 atoms) systems (single processor). ReaxFF has now been parallelized, allowing reactive simulations on >>1000,000 atoms.



: not currently described by ReaxFF

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- Initial funding for ReaxFF development was provided by the British Royal Society

More information on ReaxFF:

-Website: http://www.wag.caltech.edu/home/duin
-E-mail: duin@wag.caltech.edu